

Effective Constraints for Quantum Systems

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Abstract

An effective formalism for quantum constrained systems is presented which allows manageable derivations of solutions and observables, including a treatment of physical reality conditions without requiring full knowledge of the physical inner product. Instead of a state equation from a constraint operator, an infinite system of constraint functions on the quantum phase space of expectation values and moments of states is used. The examples of linear constraints as well as the free non-relativistic particle in parameterized form illustrate how standard problems of constrained systems can be dealt with in this framework.

1 Introduction

Effective equations are a trusted tool to sidestep some of the mathematical and conceptual difficulties of quantum theories. Quantum corrections to classical equations of motion are usually easier to analyze than the behavior of outright quantum states, and they can often be derived in a manageable way. This is illustrated, e.g., by the derivation of the low-energy effective action for anharmonic oscillators in [1] or, equivalently, effective equations for canonical quantum systems in [2, 3, 4]. But effective equations are not merely quantum corrected classical equations. They provide direct solutions for quantum properties such as expectations values or fluctuations. While semiclassical regimes play important roles in providing useful approximation schemes, effective equations present a much more general method. In fact, they may be viewed as an analysis of quantum properties independently of specific Hilbert space representation issues.

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As we will discuss here, this is especially realized for constrained systems which commonly have additional complications such as the derivation of a physical inner product or the problem of time in general relativity [5]. We therefore develop an effective constraint formalism parallel to that of effective equations for unconstrained systems. Its advantages are that (i) it avoids directly writing an integral (or other) form of a physical inner product, which is instead implemented by reality conditions for the physical variables; (ii) it shows when a phase space variable evolves classically enough to play the role of internal time which, in a precise sense, emerges from quantum gravity; and (iii) it directly provides physical quantities such as expectation values and fluctuations as relational functions of internal time, rather than computing a whole wave function first and then performing integrations. These advantages avoid conceptual problems and some technical difficulties in solving quantum equations. They can also bring out general properties more clearly, especially in quantum cosmology. Moreover, they provide equations which are more easily implemented numerically than equations for states followed by integrations to compute expectation values. (Finally, although we discuss only systems with a single classical constraint in this paper, anomaly issues can much more directly be analyzed at the effective level; see [6, 7, 8] for work in this direction.)

As we will see, however, there are still various unresolved mathematical issues for a completely general formulation. In this article, we propose the general principles behind an effective formulation of constrained systems and illustrate properties and difficulties by simple examples, including the parameterized free, non-relativistic particle where we will demonstrate the interplay of classical and quantum variables as it occurs in constrained systems. Specific procedures used in this concrete example will be general enough to encompass any non-relativistic system in parameterized form. Relativistic systems show further subtleties and will be dealt with in a forthcoming paper.

2 Setting

We first review the setup of effective equations for unconstrained Hamiltonian systems [2, 3, 4], which we will generalize to systems with constraints in the following section.

We describe a state by its moments rather than a wave function in a certain Hilbert space representation. This has the immediate advantage that the description is manifestly representation independent and deals directly with quantities of physical interest, such as expectation values and fluctuations. Just as a Hilbert space representation, the system is determined through the algebra of its basic operators and their \star -relations (adjointness or reality conditions). In terms of expectation values, fluctuations and all higher moments, this structure takes the form of an infinite dimensional phase space whose Poisson relations are derived from the basic commutation algebra. Dynamics is determined by a Hamiltonian on this phase space. As a function of all the phase space variables it is obtained by taking the expectation value of the Hamiltonian operator in a general state and expressing the state dependence as a dependence on all the moments. Thus, the Hamiltonian operator determines a function on the infinite dimensional phase space which generates Hamiltonian

evolution.¹

Specifically, for an ordinary quantum mechanical system with canonical basic operators \hat{q} and \hat{p} satisfying $[\hat{q}, \hat{p}] = i\hbar$ we have a phase space coordinatized by the expectation values $q := \langle \hat{q} \rangle$ and $p := \langle \hat{p} \rangle$ as well as infinitely many quantum variables²

$$G^{a,b} := \langle (\hat{p} - \langle \hat{p} \rangle)^a (\hat{q} - \langle \hat{q} \rangle)^b \rangle_{\text{Weyl}} \quad (1)$$

for integer a and b such that $a + b \geq 2$, where the totally symmetric ordering is used. For $a + b = 2$, for instance, this provides fluctuations $(\Delta q)^2 = G^{0,2} = G^{qq}$ and $(\Delta p)^2 = G^{2,0} = G^{pp}$ as well as the covariance $G^{1,1} = G^{qp}$. As indicated, for moments of lower orders it is often helpful to list the variables appearing as operators directly. The symplectic structure is determined through Poisson brackets which follow by the basic rule $\{A, B\} = -i\hbar^{-1} \langle [\hat{A}, \hat{B}] \rangle$ for any two operators \hat{A} and \hat{B} which define phase space functions $A := \langle \hat{A} \rangle$ and $B := \langle \hat{B} \rangle$. Moreover, for products of expectation values in the quantum variables one simply uses the Leibniz rule to reduce all brackets to the elementary ones. General Poisson brackets between the quantum variables then satisfy the formula³

$$\begin{aligned} \{G^{a,b}, G^{c,d}\} = & \sum_{r,s=0}^{\infty} \left(-\frac{1}{4}\hbar^2\right)^{r+s} \sum_{j,k} \binom{a}{j} \binom{b}{k} \binom{c}{k} \binom{d}{j} G^{a+c-j-k, b+d-j-k} (\delta_{j,2r+1} \delta_{k,2s} - \delta_{j,2r} \delta_{k,2s+1}) \\ & - adG^{a-1,b} G^{c,d-1} + bcG^{a,b-1} G^{c-1,d} \end{aligned} \quad (2)$$

where the summation of j and k is over the ranges $0 \leq j \leq \min(a, d)$ and $0 \leq k \leq \min(b, c)$, respectively. (For low order moments, it is easier to use direct calculations of Poisson brackets via expectation values of commutators.) This defines the kinematics of the quantum system formulated in terms of moments. The role of the commutator algebra of basic operators is clearly seen in Poisson brackets.

Dynamics is defined by a quantum Hamiltonian derived from the Hamiltonian operator by taking expectation values. This results in a function of expectation values and moments through the state used for the expectation value. By Taylor expansion, we have

$$\begin{aligned} H_Q(q, p, G^{a,b}) &= \langle H(\hat{q}, \hat{p})_{\text{Weyl}} \rangle = \langle H(q + (\hat{q} - q), p + (\hat{p} - p))_{\text{Weyl}} \rangle \\ &= H(q, p) + \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \frac{1}{a!b!} \frac{\partial^{a+b} H(q, p)}{\partial p^a \partial q^b} G^{a,b} \end{aligned} \quad (3)$$

¹This viewpoint in the present context of effective equations goes back to [9]. While some underlying constructions can be related to the geometrical formulation of quantum mechanics developed in [10, 11, 12], the geometrical formulation has so far not provided a rigorous derivation of effective equations. Present methods in this context remain incomplete due to a lack of treating quantum variables properly, which take center stage in the methods of [2] and those developed here. In some cases, it may be enough to place upper bounds on additional correction terms from quantum variables, based on semiclassicality assumptions. This may be done within the geometric formulation to provide *semiclassical equations* [13, 14], but it is insufficient for *effective equations*.

²Notice that the notation used here differs from that introduced in [2] because we found that the considerations of the present article, in which several canonical pairs are involved, can be presented more clearly in this way.

³We thank Joseph Ochoa for bringing a mistake in the corresponding formula of [2], as well as its correction, to our attention.

where we understand $G^{a,b} = 0$ if $a + b < 2$ and $H(q, p)$ is the classical Hamiltonian evaluated in expectation values. As written explicitly, we assume the Hamiltonian to be Weyl ordered. If another ordering is desired, it can be reduced to Weyl ordering by adding re-ordering terms.

Having a Hamiltonian and Poisson relations of all the quantum variables, one can compute Hamiltonian equations of motion $\dot{q} = \{q, H_Q\}$, $\dot{p} = \{p, H_Q\}$ and $\dot{G}^{a,b} = \{G^{a,b}, H_Q\}$. This results in infinitely many equations of motion which, in general, are all coupled to each other. This set of infinitely many ordinary differential equations is fully equivalent to the partial differential equation for a wave function given by the Schrödinger equation. In general, one can expect a partial differential equation to be solved more easily than infinitely many coupled ordinary ones. Exceptions are solvable systems such as the harmonic oscillator or the spatially flat quantum cosmology of a free, massless scalar field [15] where equations of motion for expectation values and higher moments decouple. This decoupling also allows a precise determination of properties of dynamical coherent states [16]. Such solvable systems can then be used as the basis for a perturbation theory to analyze more general systems, just like free quantum field theory provides a solvable basis for interacting ones. In quantum cosmology, this is developed in [17, 18, 19]. Moreover, semiclassical and some other regimes allow one to decouple and truncate the equations consistently, resulting in a finite set of ordinary differential equations. This is easier to solve and, as we will discuss in detail below, can be exploited to avoid conceptual problems especially in the context of constrained systems.

3 Effective constraints

For a constrained system, the definition of phase space variables (1) in addition to expectation values of basic operators is the same. For several basic variables, copies of independent moments as well as cross-correlations between different canonical pairs need to be taken into account. A useful notation, especially for two canonical pairs $(q, p; q_1, p_1)$ as we will use it later, is

$$G_{c,d}^{a,b} \equiv \langle (\hat{p} - p)^a (\hat{q} - q)^b (\hat{p}_1 - p_1)^c (\hat{q}_1 - q_1)^d \rangle_{\text{Weyl}}. \quad (4)$$

Also here we will, for the sake of clarity, sometimes use a direct listing of operators, as in $G^{qq} = G_{0,0}^{2,0} = (\Delta q)^2$ or the covariance $G_{p_1}^q = G_{1,0}^{0,1}$, for low order moments.

We assume that we have a single constraint \hat{C} in the quantum system and no true Hamiltonian; cases of several constraints or constrained systems with a true Hamiltonian can be analyzed analogously. We clearly must impose the *principal* quantum constraint $C_Q(q, p, G^{a,b}) := \langle \hat{C} \rangle = 0$ since any physical state $|\psi\rangle$, whose expectation values and moments we are computing, must be annihilated by our constraint, $\hat{C}|\psi\rangle = 0$. Just as the quantum Hamiltonian H_Q before, the quantum constraint can be written as a function of expectation values and quantum variables by Taylor expansion as in (3). However, this one condition for the phase space variables is much weaker than imposing a Dirac constraint on states, $\hat{C}|\psi\rangle = 0$. In fact, a simple counting of degrees of freedom shows that

additional constraints must be imposed: One classical constraint such as $C = 0$ removes a pair of canonical variables by restricting to the constraint surface and factoring out the flow generated by the constraint. For a quantum system, on the other hand, we need to eliminate infinitely many variables such as a canonical pair (q, p) together with all the quantum variables it defines. Imposing only $C_Q = 0$ would remove a canonical pair but leave all its quantum variables unrestricted. These additional variables are to be removed by infinitely many further constraints.

There are obvious candidates for these constraints. If $\hat{C}|\psi\rangle = 0$ for any physical state, we do not just have a single constraint $\langle\hat{C}\rangle = 0$ but infinitely many *quantum constraints*

$$C^{(n)} := \langle\hat{C}^n\rangle = 0 \quad (5)$$

$$C_{f(q,p)}^{(n)} := \langle f(\hat{q}, \hat{p})\hat{C}^n \rangle = 0 \quad (6)$$

for positive integer n and arbitrary phase space functions $f(q, p)$. All these expectation values vanish for physical states, and in general differ from each other on the quantum phase space. For arbitrary $f(q, p)$, there is an uncountable number of constraints which should be restricted suitably such that a closed system of constraints results which provides a complete reduction of the quantum phase space. The form of functions $f(q, p)$ to be included in the quantum constraint system depends on the form of the classical constraint and its basic algebra. Examples and a general construction scheme are presented below.

We thus have indeed infinitely many constraints,⁴ which constitute the basis for our effective constraints framework. This is to be solved as a classical constrained system, but as an infinite one on an infinite dimensional phase space. An effective treatment then requires approximations whose explicit form depends on the specific constraints. At this point, some caution is required: approximations typically entail disregarding quantum variables beyond a certain order to make the system finite. Doing so for an order of moments larger than two results in a Poisson structure which is not symplectic because only the expectation values form a symplectic submanifold of the full quantum phase space, but no set of moments to a certain order does. We are then dealing with constrained systems on Poisson manifolds such that the usual countings of degrees of freedom do not apply. For instance, it is not guaranteed that each constraint generates an independent flow even if it weakly commutes with all other constraints which would usually make it first class. Properties of constrained systems in the more general setting of Poisson manifolds which need not be symplectic are discussed, e.g., in [21].

⁴As observed in [20], a single constraint $C^{(2)}$ would guarantee a complete reduction for a system where zero is in the discrete part of the spectrum of a self-adjoint \hat{C} . In this case, non-degeneracy of the inner product ensures that $\langle\psi|\hat{C}^2|\psi\rangle = 0$ implies $\hat{C}|\psi\rangle = 0$. However, details of the quantization and the quantum representation are required for this conclusion, based also on properties of the spectrum, which is against the spirit of effective equations. Moreover, the resulting constraint equation $C^{(2)}$ is in general rather complicated and must be approximated for explicit analytical or numerical solutions. Then, if $C^{(2)} = 0$ is no longer imposed exactly, a large amount of freedom for uncontrolled deviations from $\hat{C}|\psi\rangle = 0$ would open up. In our approach, we are using more than one constraint which ensures that even under approximations the system remains sufficiently well controlled. Moreover, our considerations remain valid for constraints with zero in the continuous parts of their spectra, although as always there are additional subtleties.

We also emphasize that gauge flows generated by quantum constraints on the quantum phase space play important roles, which one may not have expected from the usual Dirac treatment of constraints. There, only a constraint equation is written for states, but no gauge flow on the Hilbert space needs to be factored out. In fact, the gauge flow which one could define by $\exp(it\hat{C})|\psi\rangle$ for a self-adjoint \hat{C} trivializes on physical states which solve the constraint equation $\hat{C}|\psi\rangle = 0$. In the context of effective constraints, there are two main reasons why the gauge flow does not trivialize and becomes important for a complete removal of gauge dependent variables: First, to define the gauge flow $\exp(it\hat{C})|\psi\rangle$ and conclude that it trivializes on physical states, one implicitly uses self-adjointness of \hat{C} and assumes that physical states are in the kinematical Hilbert space for otherwise it would not be the original \hat{C} that could be used in the flow. These are specific properties of the kinematical representation which we are not making use of in the effective procedure used here, where reality and normalization conditions are not imposed before the very end of finding properties of states in the physical Hilbert space. The expectation values and moments we are dealing with when imposing quantum constraints thus form a much wider manifold than the Hilbert space setting would allow. Here, not only constraint equations but also gauge flows on the constraint surface are crucial. If representation properties are given which imply that physical states are in the kinematical Hilbert space, we will indeed see that the flow trivializes as the example in Sec. 4.2 shows. Secondly, the Dirac constraint $\hat{C}|\psi\rangle = 0$ corresponds to infinitely many conditions, and only when all of them are solved can the gauge-flow trivialize. An effective treatment, on the other hand, shows its strength especially when one can reduce the required set of equations to finitely many ones, which in our case would imply only a partial solution of the Dirac constraint. On these partial solutions, which for instance make sure that fluctuations correspond to those of a state satisfying $\hat{C}|\psi\rangle = 0$ even though other moments do not need to come from such a state, the gauge-flow does not trivialize.

We will illustrate such properties as well as solution schemes of effective constraints in examples below. But there are also general conclusions which can be drawn. As the main requirements, we have to ensure the system of effective constraints to be consistent and complete. Consistency means that the set of all constraints should be first class if we start with a single classical constraint or a first class set of several constraints. As we will illustrate by examples, this puts restrictions on the form of quantum constraints, related to the ordering of operators used, beyond the basic requirement that they be zero when computed in physical states.

To show that the constraints are complete, i.e. they remove all expectation values and quantum variables associated with one canonical pair, we will consider a constraint $\hat{C} = \hat{q}$ in Sec. 4.1. Since locally one can always choose a single (irreducible) constraint to be a phase space variable, this will serve as proof that local degrees of freedom are reduced correctly. (Still, global issues may pose non-trivialities since entire gauge orbits must be factored out when constraints are solved.)

3.1 The form of quantum constraints

At first sight, our definition of quantum constraints may seem problematic. Some of them in (6) are defined as expectation values of non-symmetric operators, thus implying complex valued constraint functions. (We specifically do not order symmetrically in (6) because this would give rise to terms where some \hat{q} or \hat{p} appear to the right while others remain to the left. This would not vanish for physical states and therefore not correspond to a constraint.) This may appear problematic, but one should note that this reality statement is dependent on the (kinematical) inner product used before the constraints are imposed. This inner product in general differs from the physical one if zero is in the continuous part of the spectrum of the constraint and thus reality in the kinematical inner product is not physically relevant. Moreover, in gravitational theories it is common or even required to work with constraint operators which are not self-adjoint [22], and thus complex valued constraints have to be expected in general. For physical statements, which are derived after the constraints have been implemented, only the final reality conditions of the physical inner product are relevant.⁵

As we will discuss in more detail later, this physical reality can be implemented effectively: We solve the constraints on the quantum phase space, and then impose the condition that the reduced quantum phase space be real. We will see explicitly that complex-valued quantum variables on the unconstrained phase space are helpful to ensure consistency. In parallel to Hilbert space notation, we call quantum variables (1) on the original quantum phase space *kinematical quantum variables*, and those on the reduced quantum phase space *physical quantum variables*. Kinematical quantum variables are allowed to take complex values because their reality would only refer to the inner product used on the kinematical Hilbert space. For physical quantum variables in the physical Hilbert space as usually defined, on the other hand, reality conditions must be imposed.

3.1.1 Closure of constrained system

Still, it may seem obvious how to avoid the question of reality of the constraints altogether by using quantum constraints defined as $G^{C^n f(q,p)} = \langle \hat{C}^n \widehat{f(p,q)} \rangle_{\text{Weyl}}$ such as $G^{C^n q}$ and $G^{C^n p}$ with the symmetric ordering used as in (1). Here, the symmetric ordering contained in the definition of quantum variables must leave \hat{C} intact as a possibly composite operator, i.e. we have for instance $G^{C,p} = \frac{1}{2} \langle \hat{C} \hat{p} + \hat{p} \hat{C} \rangle - Cp$ independently of the functional form of \hat{C} in terms of \hat{q} and \hat{p} . Otherwise it would not be guaranteed that the expectation value vanishes on physical states. We could not include variables with higher powers of q and p , such as $G^{C^n pp}$ as constraints because there would be terms in the totally symmetric ordering (such as $\hat{p} \hat{C}^n \hat{p}$) not annihilating a physical state. But, e.g., $G^{\hat{C} \hat{p}^2}$ understood as $\frac{1}{2} \langle \hat{C} \hat{p}^2 + \hat{p}^2 \hat{C} \rangle - Cp^2$ would be allowed. The use of such symmetrically ordered variables would imply real quantum constraints.

⁵At least partially, the meaning of reality conditions depends on specifics of the measurement process. This may be further reason to keep an open mind toward reality conditions especially in quantum gravity.

However, this procedure is not feasible: The constraints would not form a closed set and not even be first class. We have, for instance,

$$\begin{aligned} \{G^{C^n, f(q,p)}, G^{C^m, g(q,p)}\} &= \frac{1}{4i\hbar} \langle [\hat{C}^n \hat{f} + \hat{f} \hat{C}^n, \hat{C}^m \hat{g} + \hat{g} \hat{C}^m] \rangle \\ &\quad - \frac{g}{2i\hbar} \langle [\hat{C}^n \hat{f} + \hat{f} \hat{C}^n, \hat{C}^m] \rangle - \frac{C^m}{2i\hbar} \langle [\hat{C}^n \hat{f} + \hat{f} \hat{C}^n, \hat{g}] \rangle \\ &\quad - \frac{f}{2i\hbar} \langle [\hat{C}^m, \hat{C}^m \hat{g} + \hat{g} \hat{C}^m] \rangle - \frac{C^n}{2i\hbar} \langle [\hat{f}, \hat{C}^m \hat{g} + \hat{g} \hat{C}^m] \rangle \\ &\quad + \{C^n f, C^m g\}. \end{aligned}$$

The first commutator contains several terms which vanish when the expectation value is taken in a physical state, but also the two contributions $[\hat{C}^n, \hat{g}] \hat{C}^m \hat{f}$ and $\hat{f} \hat{C}^m [\hat{C}^n, \hat{g}]$ whose expectation value in a physical state vanishes only if \hat{f} or \hat{g} commute with \hat{C} . This would require quantum observables to be known and used in the quantum constraints, which in general would be too restrictive and impractical.

By contrast, the quantum constraints defined above do form a first class system: We have

$$[\hat{f} \hat{C}^n, \hat{g} \hat{C}^m] = [\hat{f}, \hat{g}] \hat{C}^{n+m} + \hat{f} [\hat{C}^n, \hat{g}] \hat{C}^m + \hat{g} [\hat{f}, \hat{C}^m] \hat{C}^n \quad (7)$$

whose expectation value in any physical state vanishes. Thus, using these constraints implies that their quantum Poisson brackets vanish on the constraint surface, providing a weakly commuting set:

$$\{C_f^{(n)}, C_g^{(m)}\} = \frac{1}{i\hbar} \langle [\hat{f} \hat{C}^n, \hat{g} \hat{C}^m] \rangle \approx 0. \quad (8)$$

A further possibility of using Weyl-ordered constraints of a specific form will be discussed briefly in Sec. 3.2, but also this appears less practical in concrete examples than using non-symmetrized constraints.

Constraints thus result for all phase space functions $f(q, p)$, but not all constraints in this uncountable set can be independent. For practical purposes, one would like to keep the number of allowed functions to a minimum while keeping the system complete. Then, however, the set of quantum constraints is not guaranteed to be closed for any restricted choice of phase space functions in their definition. If $C_f^{(n)}$ and $C_g^{(m)}$ are quantum constraints, closure requires the presence of $C_{[f,g]}^{(n)}$ (for $n \geq 2$), $C_{f[C^m, g]}^{(n)}$ and $C_{g[C^m, f]}^{(n)}$ as additional constraints according to (7). This allows the specification of a construction procedure for a closed set of quantum constraints. As we will see in examples later, for a system in canonical variables (q, p) it is necessary to include at least $C_q^{(n)}$ and $C_p^{(m)}$ in the set of constraints for a complete reduction. With $C_{[q,p]}^{(n)} = i\hbar C^{(n)}$, the first new constraints resulting from a closed constraint algebra add nothing new. However, in general the new constraints $C_{q[C^m, p]}^{(n)}$ and $C_{p[C^m, q]}^{(n)}$ will be independent and have to be included. Iteration of the procedure generates further constraints in a process which may or may not stop after finitely many steps depending on the form of the classical constraint.

Although many independent constraints have to be considered for a complete system, most of them will involve quantum variables of a high degree. To a given order in the moments it is thus sufficient to consider only a finite number of constraints which can be determined and analyzed systematically. Such truncations and approximations will be discussed by examples in Secs. 5 and 6.

3.1.2 Number of effective constraints: linear constraint operator

For special classes of constraints one can draw further conclusions at a more general level. In particular for a linear constraint, which shows the local behavior of singly constrained systems, it is sufficient to consider polynomial multiplying functions as we will justify by counting degrees of freedom. Because this counting depends on the number of degrees of freedom, we generalize, in this section only, our previous setting to a quantum system of $N + 1$ canonical pairs of operators $(\hat{q}^i, \hat{p}_i)_{i=1, \dots, N+1}$ satisfying the usual commutation relations $[\hat{q}^i, \hat{p}_j] = i\hbar\delta_j^i$. Furthermore, it is sufficient to consider only the case where the constraint itself is one of the canonical variables. Given any constraint operator \hat{C} , linear in the canonical variables, we can always find linear combinations of the canonical operators $((\hat{x}_i)_{i=1, \dots, N}; \hat{q}, \hat{p})$ such that $\hat{q} = \hat{C}$ and

$$[\hat{q}, \hat{p}] = i\hbar \quad , \quad [\hat{q}, \hat{x}_i] = [\hat{p}, \hat{x}_i] = 0 \quad , \quad [\hat{x}_i, \hat{x}_j] = i\hbar(\delta_{i,j-N} - \delta_{i-N,j})$$

i.e. \hat{x}_i form an algebra of N canonical pairs ($i = 1, \dots, N$ and $i = N + 1, \dots, 2N$ corresponding to the configuration and momentum operators, respectively).⁶ For the rest of this subsection we assume the above notation, so that our quantum system is parameterized by the expectation values $q := \langle \hat{q} \rangle$, $p := \langle \hat{p} \rangle$, $x_i := \langle \hat{x}_i \rangle$, $i = 1, \dots, 2N$ and the quantum variables:

$$G^{a_1, a_2, \dots, a_{2N}; b, c} := \langle (\hat{x}_1 - x_1)^{a_1} \cdots (\hat{x}_{2N} - x_{2N})^{a_{2N}} (\hat{p} - p)^b (\hat{q} - q)^c \rangle_{\text{Weyl}} \quad (9)$$

where the operator product is totally symmetrized.

As proposed, we include among the constraints all functions of the form $C_f = \langle \hat{f}\hat{C} \rangle$, where \hat{f} is now any operator polynomial in the canonical variables. This proposition is consistent with $\hat{C}|\psi\rangle = 0$ and the set of operators of the form $\hat{f}\hat{C}$ is closed under taking commutators. As a result the set of all such functions C_f is first-class with respect to the Poisson bracket induced by the commutator. ($C_f^{(n)}$ is automatically included in the above constraints through $C_{f'}$ where $\hat{f}' = \hat{f}\hat{C}^{n-1}$, which is polynomial in the canonical variables so long as \hat{f} is.)

In principle, we have an infinite number of constraints to restrict an infinite number of quantum variables. To see how the degrees of freedom are reduced, we proceed order by order. Variables of the order M in $N + 1$ canonical pairs are defined as in Eq. (9), with

⁶The linear combinations that would satisfy the above relations may be obtained by performing a linear canonical transformation on the operators (post-quantization). Such combinations are not unique, but this fact is not important for the purpose of counting the degrees of freedom.

$\sum_i a_i + b + c = M$. The total number of different combinations of this form is the same as the number of ways the positive powers adding up to M can be distributed between $2(N+1)$ terms, that is $\binom{M+2(N+1)-1}{2(N+1)-1}$. Solving a single constraint classically results in the (local) removal of one canonical pair. Subsequent quantization of the theory would result in quantum variables corresponding to N canonical pairs. In the rest of the section we demonstrate that our selected form of the constraints leaves unrestricted precisely the quantum variables of the form $G^{a_1, \dots, a_{2N}; 0, 0}$.

It is convenient to make another change in variables. We note that in order to permute two non-commuting canonical operators in a product we need to add $i\hbar$ times a lower order product. Starting with a completely symmetrized product of order M and iterating the procedure we can express it in terms of a sum of unsymmetrized products of orders M and below, in some pre-selected order. In particular, we consider variables of the form:

$$F^{a_1, a_2, \dots, a_{2N}; b, c} := \langle (\hat{x}_1)^{a_1} \cdots (\hat{x}_{2N})^{a_{2N}} \hat{p}^b \hat{q}^c \rangle \quad (10)$$

It is easy to see that there is a one-to-one correspondence between variables (9) (combined with the expectation values) and (10), but the precise mapping is tedious to derive and not necessary for counting. We can immediately see that our constraints require $F^{a_1, a_2, \dots, a_{2N}; b, c} \approx 0$ for $c \neq 0$. Moreover, all of the constraints $C_f = \langle \hat{f} \hat{C} \rangle$ may be written as a combination of the variables $F^{a_1, a_2, \dots, a_{2N}; b, c}$, $c \neq 0$ (again, this can be seen by noting that we may rearrange the order of operators in a product by adding terms proportional to lower order products). There are still too many degrees of freedom left as none of the variables $F^{a_1, a_2, \dots, a_{2N}; b, 0}$ are constrained.

At this point, however, we are yet to account for the unphysical degrees of freedom associated with the gauge transformations. Indeed, every constraint induces a flow on the space of quantum variables through the Poisson bracket, associated with the commutator of the algebra of canonical operators. The set of constraints C_f is first-class, which means that the flows they produce preserve constraints and are therefore tangent to the constraint surface. However, not all of the flow-generating vector fields corresponding to the distinct constraints considered above will be linearly independent on the constraint surface because, to a fixed order in moments, we are dealing with a non-symplectic Poisson manifold. The degeneracy becomes obvious when we count the degrees of freedom to a given order. To order M the constraints are accounted for by variables $F^{a_1, a_2, \dots, a_{2N}; b, c+1}$, where $\sum_i a_i + b + c + 1 = M$. Counting as earlier in the section, there are $\binom{M+2(N+1)-2}{2(N+1)-1}$ such variables. Subtracting the number of constraints from the number of quantum variables of order M , we are left with

$$\begin{aligned} & \binom{M+2(N+1)-1}{2(N+1)-1} - \binom{M+2(N+1)-2}{2(N+1)-1} \\ &= \left(\frac{M+2(N+1)-1}{M+2(N+1)-1-(2N+1)} - 1 \right) \binom{M+2(N+1)-2}{2(N+1)-1} \\ &= \frac{2(N+1)-1}{M} \binom{M+2(N+1)-2}{2(N+1)-1} \end{aligned} \quad (11)$$

unrestricted quantum variables. If each constraint does generate an independent non-vanishing flow, we should subtract the number of constraints from the result again to get $\frac{2(N+1)-1-M}{M} \binom{M+2(N+1)-2}{2(N+1)-1}$ physical degrees of freedom of order M . This number becomes negative once M is large enough raising the possibility that the system has been over-constrained.

Fortunately, this is not the case. All of the operators \hat{x}_i commute with the original constraint operator $\hat{C}(\equiv \hat{q})$, which means that any function of the expectation value of a polynomial in $(\hat{x}_i)_{i=1,\dots,2N}$; $g = \langle g[\hat{x}_i] \rangle$, weakly commutes with every constraint

$$\{C_f, \langle g[\hat{x}_i] \rangle\} = \frac{1}{i\hbar} \left\langle [\hat{f}\hat{C}, g[\hat{x}_i]] \right\rangle = \frac{1}{i\hbar} \left\langle \hat{f} [\hat{C}, g[\hat{x}_i]] + [\hat{f}, g[\hat{x}_i]] \hat{C} \right\rangle = \frac{1}{i\hbar} \left\langle [\hat{f}, g[\hat{x}_i]] \hat{C} \right\rangle \quad (12)$$

which vanishes on the constraint surface. This means that the variables $F^{a_1, a_2, \dots, a_{2N}; 0, 0}$ are both unconstrained and unaffected by the gauge flows. They can be used to construct the quantum variables corresponding to precisely N canonical pairs, so that we have *at least* the correct number of physical degrees of freedom. Finally we show that the variables $F^{a_1, a_2, \dots, a_{2N}; b, 0}$, $b \neq 0$ are *pure gauge*

$$\begin{aligned} \{C_f, F^{a_1, a_2, \dots, a_{2N}; b, 0}\} &= \frac{1}{i\hbar} \left\langle [\hat{f}\hat{C}, (\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}} \hat{p}^b] \right\rangle \\ &= \frac{1}{i\hbar} \left\langle [\hat{f}, (\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}} \hat{p}^b] \hat{C} + i\hbar b \hat{f} (\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}} \hat{p}^{b-1} \right\rangle \\ &\approx b \left\langle \hat{f} (\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}} \hat{p}^{b-1} \right\rangle \end{aligned} \quad (13)$$

where “ \approx ” denotes equality on the constraint surface. Substituting a constraint such that $\hat{f} = g[\hat{x}_i] \hat{C}^{b-1}$

$$\{C_{g\hat{C}^{b-1}}, F^{a_1, a_2, \dots, a_{2N}; b, 0}\} \approx b \left\langle g[\hat{x}_i] ((\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}}) \hat{C}^{b-1} \hat{p}^{b-1} \right\rangle$$

and commuting all the \hat{C} to the right one by one, such that $\hat{C}^{b-1} \hat{p}^{b-1} = (b-1)!(i\hbar)^{b-1} + \dots$ up to operators of the form $\hat{A}\hat{C}$, we have

$$\{C_{g\hat{C}^{b-1}}, F^{a_1, a_2, \dots, a_{2N}; b, 0}\} \approx b!(i\hbar)^{b-1} \left\langle g[\hat{x}_i] ((\hat{x}_1)^{a_1} \dots (\hat{x}_{2N})^{a_{2N}}) \right\rangle. \quad (14)$$

Since the right-hand side is a gauge independent function, (14) tells us that it is impossible to pick a gauge where all of the flows on a given variable $F^{a_1, a_2, \dots, a_{2N}; b, 0}$ vanish, in this sense we refer to all such variables as *pure gauge*.

To summarize: using an alternative set of variables $F^{a_1, a_2, \dots, a_{2N}; b, c}$ defined in Eq. (10) we find that constraints become $F^{a_1, a_2, \dots, a_{2N}; b, c} \approx 0$, $c \neq 0$; the variables $F^{a_1, a_2, \dots, a_{2N}; b, 0}$, $b \neq 0$ are pure gauge, which leaves the gauge invariant and unconstrained physical variables $F^{a_1, a_2, \dots, a_{2N}; 0, 0}$. These may then be used to determine directly the physical quantum variables $G^{a_1, \dots, a_{2N}; 0, 0}$ defined in Eq. (9). Thus, for a linear constraint a correct reduction in the degrees of freedom is achieved by applying constraints of the form $C_f = \langle \hat{f}\hat{C} \rangle$ (polynomial in the canonical variables), as can be directly observed order by order in the quantum variables. Locally, our procedure of effective constraints is complete and consistent since any irreducible constraint can locally be chosen as a canonical coordinate.

3.2 Generating functional

More generally, one can work with a generating functional of all constraints with polynomial-type multipliers, which can then be extended to arbitrary constraints including non-linear ones.

To elaborate, we return to a single canonical pair and denote basic operators as $(\hat{x}^i)_{i=1,2} = (\hat{q}, \hat{p})$ such that they satisfy the Heisenberg algebra $[\hat{x}^i, \hat{x}^j] = i\hbar\epsilon^{ij}$, where ϵ^{ij} are the components of the non-degenerate antisymmetric tensor with $\epsilon^{12} = 1$. We assume that there is a Weyl ordered constraint operator $C(\hat{x}^i)$ obtained by inserting the basic operators in the classical constraint and then Weyl ordering. We can generate the Weyl ordered form of all quantum constraints and their algebra through use of a generating functional, defining $C_\alpha(\hat{x}^i) := e^{\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i} C(\hat{x}^i)$ for all $\alpha_i \in \mathbb{R}$, which turn out to form a closed algebra. It is clear that $\langle C_\alpha(\hat{x}^i) \rangle = 0$ for physical states, and thus we have a specific class of infinitely many quantum constraints. This class includes polynomials as multipliers which arise from

$$\langle \hat{q}^a \hat{p}^b \hat{C} \rangle \propto \left(\frac{\partial^{a+b}}{\partial \alpha_1^a \partial \alpha_2^b} \langle C_\alpha(\hat{x}^i) \rangle \right) \Big|_{\alpha=0}$$

in specific orderings as Weyl ordered versions of $\hat{q}^a \hat{p}^b \hat{C}$ such that expectation values remain zero in physical states because $\langle C_\alpha(\hat{x}^i) \rangle = 0$ for all α . From Sec. 3.1.1 one may suspect that this system is not closed, but closure does turn out to be realized. To establish this, we provide several auxiliary calculations. First, we have

$$\begin{aligned} [\hat{x}^{(i_1 \dots i_n)}, \hat{x}^j]_+ &= \frac{1}{2} \delta_{(j_1}^{i_1} \dots \delta_{j_n)}^{i_n} (\hat{x}^{j_1} \dots \hat{x}^{j_n} \hat{x}^j + \hat{x}^j \hat{x}^{j_1} \dots \hat{x}^{j_n}) \\ &= \frac{1}{2(n+1)} \delta_{(j_1}^{i_1} \dots \delta_{j_n)}^{i_n} \left[2 \sum_{r=0}^n \hat{x}^{j_1} \dots \hat{x}^{j_r} \hat{x}^j \hat{x}^{j_{r+1}} \dots \hat{x}^{j_n} \right. \\ &\quad + \sum_{r=1}^n i\hbar(n+1-r) \epsilon^{jj_r} \hat{x}^{j_1} \dots \hat{x}^{j_{r-1}} \hat{x}^{j_{r+1}} \dots \hat{x}^{j_n} \\ &\quad \left. + \sum_{r=1}^n i\hbar(n+1-r) \epsilon^{j_{n-r}j} \hat{x}^{j_1} \dots \hat{x}^{j_{n-r-1}} \hat{x}^{j_{n-r+1}} \dots \hat{x}^{j_n} \right] \\ &= \hat{x}^{(i_1 \dots i_n} \hat{x}^{j)}. \end{aligned} \tag{15}$$

Thus, the anticommutator of a Weyl ordered operator with a basic operator is also Weyl ordered.

From Baker–Campbell–Hausdorff identities it follows that $e^{\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i}$ acts as a displacement operator

$$e^{\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i} \hat{x}^j e^{-\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i} = \hat{x}^j + \epsilon^{ji} \alpha_i. \tag{16}$$

This also shows the algebra of these operators:

$$e^{\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i} e^{\frac{i}{\hbar}\beta_i \cdot \hat{x}^i} = e^{\frac{i}{\hbar}\alpha_i \cdot \hat{x}^i + \frac{i}{\hbar}\beta_i \cdot \hat{x}^i - \frac{1}{2\hbar^2} [\alpha \cdot \hat{x}, \beta \cdot \hat{x}]} = e^{\frac{i}{\hbar}(\alpha_i + \beta_i) \cdot \hat{x}^i} e^{-\frac{i}{2\hbar} \alpha_i \epsilon^{ij} \beta_j}. \tag{17}$$

With this, one can realize the operator $C_\alpha(\hat{x}^i)$ as

$$\begin{aligned}
C_\alpha(\hat{x}^i) &:= e^{\frac{i}{\hbar}\alpha_i\hat{x}^i}C(\hat{x}^i) = e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i}C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}\alpha_j)e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i} \\
&= \sum_{n=0}^{\infty} \sum_{m=0}^n \frac{1}{2^n \hbar^n n!} \binom{n}{m} (i\alpha \cdot \hat{x})^m C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}\alpha_j) (i\alpha \cdot \hat{x})^{n-m} \\
&= \sum_{n=0}^{\infty} \frac{1}{\hbar^n n!} [i\alpha \cdot \hat{x}, C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}\alpha_j)]_{+n},
\end{aligned} \tag{18}$$

which is manifestly Weyl ordered due to (15). Here, we use the iterative definition $[\hat{A}, \hat{C}]_{+0} := \hat{C}$ and $[\hat{A}, \hat{C}]_{+n} := [\hat{A}, [\hat{A}, \hat{C}]]_{+(n-1)}$.

Finally, the algebra of constraints is

$$\begin{aligned}
[C_\alpha(\hat{x}^i), C_\beta(\hat{x}^i)] &= \left(e^{\frac{i}{\hbar}\alpha_i\hat{x}^i}C(\hat{x}^i)e^{\frac{i}{\hbar}\beta_i\hat{x}^i} - e^{\frac{i}{\hbar}\beta_i\hat{x}^i}C(\hat{x}^i)e^{\frac{i}{\hbar}\alpha_i\hat{x}^i} \right) C(\hat{x}^i) \\
&= \left(e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i}C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}\alpha_j)e^{\frac{i}{\hbar}\beta_i(\hat{x}^i + \frac{1}{2}\epsilon^{ij}\alpha_j)}e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i} \right. \\
&\quad \left. - e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i}e^{\frac{i}{\hbar}\beta_i(\hat{x}^i - \frac{1}{2}\epsilon^{ij}\alpha_j)}C(\hat{x}^i - \frac{1}{2}\epsilon^{ij}\alpha_j)e^{\frac{i}{2\hbar}\alpha_i\hat{x}^i} \right) C(\hat{x}^i) \\
&= \left(e^{\frac{i}{\hbar}\beta_i\frac{1}{2}\epsilon^{ij}\alpha_j}e^{\frac{i}{2\hbar}(\alpha_i+\beta_i)\hat{x}^i}C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}(\alpha_j - \beta_j))e^{\frac{i}{2\hbar}(\alpha_i+\beta_i)\hat{x}^i} \right. \\
&\quad \left. - e^{-\frac{i}{\hbar}\beta_i\frac{1}{2}\epsilon^{ij}\alpha_j}e^{\frac{i}{2\hbar}(\alpha_i+\beta_i)\hat{x}^i}C(\hat{x}^i - \frac{1}{2}\epsilon^{ij}(\alpha_j - \beta_j))e^{\frac{i}{2\hbar}(\alpha_i+\beta_i)\hat{x}^i} \right) C(\hat{x}^i)
\end{aligned} \tag{19}$$

$$\tag{20}$$

and thus

$$\begin{aligned}
[C_\alpha(\hat{x}^i), C_\beta(\hat{x}^i)] &= \left[e^{\frac{i}{2\hbar}\beta_i\epsilon^{ij}\alpha_j}C(\hat{x}^i + \frac{1}{2}\epsilon^{ij}(\alpha_j - \beta_j)) \right. \\
&\quad \left. - e^{-\frac{i}{2\hbar}\beta_i\epsilon^{ij}\alpha_j}C(\hat{x}^i - \frac{1}{2}\epsilon^{ij}(\alpha_j - \beta_j)) \right] C_{\alpha+\beta}(\hat{x}^i).
\end{aligned} \tag{21}$$

This produces a closed set of Weyl ordered and thus real effective constraints, which is uncountable. There are closed subsets obtained by allowing α_i to take values only in a lattice in phase space, but in this case the completeness issue becomes more difficult to address. Moreover, the C_α may be difficult to compute in specific examples. At this stage, we turn to a discussion of specific examples based on polynomial multipliers in quantum constraints, rather than providing further general properties of Weyl ordered effective constraints.

4 Linear examples

Given that the precise implementation of a set of quantum constraints depends on the form of the constrained system, we illustrate typical properties by examples, starting with linear ones.

4.1 A canonical variable as constraint: $\hat{C} = \hat{q}$

From $C^{(n)} = 0$ we obtain that all quantum variables G^{q^n} are constrained to vanish, in addition to $C_Q = q$ itself. Moreover, $C_q^{(n)} = C^{(n+1)}$ is already included, and $C_p^{(n)} = \langle \hat{p} \hat{q}^n \rangle$ provides a closed set of constraints. In fact, computing commutators does not add any new constraints and we already have a closed, first class system which suffices to discuss moments up to second order. At higher orders, also $C_{p^m}^{(n)} = \langle \hat{p}^m \hat{q}^n \rangle$ must be included.

In this example, it is feasible to work with the symmetrically ordered quantum variables since there is an obvious quantum observable \hat{q} commuting with the constraint. For instance, quantum variables $G^{C^n q}$ and $G^{C^n p}$ form a closed set of constraints as shown by the previous calculations. The first class nature of this system can directly be verified from the Poisson relations (2). For $b = d = 0$ we obviously have $\{G^{a,0}, G^{c,0}\} = 0$, for $b = 0$ and $d = 1$ we have $\{G^{a,0}, G^{c,1}\} = a(G^{a+c-1,0} - G^{a-1,0}G^{c,0}) \approx 0$ and for $b = d = 1$, $\{G^{a,1}, G^{c,1}\} = (a - c)G^{a+c-1,1} - aG^{a-1,1}G^{c,0} + cG^{a,0}G^{c-1,1} \approx 0$.

To discuss moments up to second order, constraints with at most a single power of p are needed. These constraints are in fact equivalent to constraints given by quantum variables due to

$$\begin{aligned}
G^{q^n} &= \langle (\hat{q} - q)^n \rangle = \sum_{j=0}^n \binom{n}{j} (-1)^j q^j \langle \hat{q}^{n-j} \rangle = \sum_{j=0}^{n-1} \binom{n}{j} (-1)^j q^j C^{(n-j)} + (-1)^n q^n \quad (22) \\
G^{q^n p} &= \frac{1}{n+1} \langle (\hat{q} - q)^n (\hat{p} - p) + (\hat{q} - q)^{n-1} (\hat{p} - p) (\hat{q} - q) + \cdots + (\hat{p} - p) (\hat{q} - q)^n \rangle \\
&= \frac{1}{n+1} \langle (n+1) (\hat{p} - p) (\hat{q} - q)^n + \frac{1}{2} i n (n+1) \hbar (\hat{q} - q)^{n-1} \rangle \\
&= \langle \hat{p} \hat{q}^n \rangle - p \langle (\hat{q} - q)^n \rangle + \sum_{j=1}^n \binom{n}{j} (-1)^j q^j \langle \hat{p} \hat{q}^{n-j} \rangle + \frac{1}{2} i n \hbar \langle (\hat{q} - q)^{n-1} \rangle \\
&= C_p^{(n)} - p G^{q^n} + \sum_{j=1}^{n-1} \binom{n}{j} (-1)^j q^j C_p^{(n-j)} + (-1)^n q^n p + \frac{1}{2} i \hbar n G^{q^{n-1}}. \quad (23)
\end{aligned}$$

This describes a one-to-one mapping from $\{C^{(n)}, C_p^{(m-1)}\}_{n,m \in \mathbb{N}}$ to $\{G^{q^n}, G^{q^m p}\}_{n,m \in \mathbb{N}}$ which provides specific examples of the relation between (9) and (10) in Sec. 3.1.2. Thus, the constraint surface as well as the gauge flow can be analyzed using quantum variables. For this type of classical constraint, reordering will only lead to either a constant or to terms depending on quantum variables defined without reference to \hat{p} . Since these are already included in the set of constraints and a constant does not matter for generating canonical transformations, they can be eliminated when computing the gauge flow. Note, however, that there is a constant term $\frac{1}{2} i \hbar$ in $G^{q^n p}$ for $n = 1$ which will play an important role in determining the constraint surface. The fact that constraints are complex valued does not pose a problem for the gauge flow since imaginary contributions come only with coefficients which are (real) constraints themselves and thus vanish weakly, or are constant and thus irrelevant for the flow.

Also the gauge flow up to second order generated by the quantum constraints can be computed using quantum variables such as G^{q^n} and $G^{q^n p}$ rather than the non-symmetric version. For the moments of different orders, we then have the following constraints and gauge transformations. (i) Expectation values: one constraint $q \approx 0$ generating one gauge transformation $p \mapsto p + \lambda_1$. (ii) Fluctuations: two constraints $G^{qq} \approx 0$ and $G^{qp} \approx \text{const}$, generating gauge transformations $G^{pp} \mapsto G^{pp} + 4\lambda_2 G^{qp}$ and $G^{pp} \mapsto G^{pp}(1 + 2\lambda_2)$, respectively. As we will see in Eq. (24) below, G^{qp} is non-zero on the constraint surface, such that G^{pp} is completely gauge. (iii) Higher moments: at each order, we have constraints $C_{p^m}^{(n-m)}$ with $m < n$ and only G^{p^n} is left to be removed by gauge generated e.g. by G^{q^n} . This confirms the counting of Sec. 3.1.2. Moreover, higher order constraints generate a gauge flow which also affects fluctuations, in particular G^{pp} . Thus, to second order we see that two moments are eliminated by quantum constraints while the remaining one is gauge. In this way, the quantum variables are eliminated completely either by constraints or by being pure gauge. (Moments such as G^{qp} were not included in the counting argument of Sec. 3.1.2 in the context of the dimension of the gauge flow to be factored out. Here, in fact, we verify that the flow generated by G^{qq} suffices to factor out all remaining quantum variables to second order.)

This example also illustrates nicely the role of imaginary contributions to the constraints from the perspective of the kinematical inner product. The constraint $C_p^{(1)} = \langle \hat{p}\hat{q} \rangle = 0$ implies that

$$G^{qp} = \frac{1}{2} \langle \hat{q}\hat{p} + \hat{p}\hat{q} \rangle - qp = \langle \hat{p}\hat{q} \rangle - qp + \frac{1}{2}i\hbar \approx \frac{1}{2}i\hbar \quad (24)$$

must be imaginary. From the point of view of the kinematical inner product this seems problematic since we are taking the expectation value of a symmetrically ordered product of self-adjoint operators. However, the inner product of the kinematical Hilbert space is only auxiliary, and from our perspective not even necessary to specify. Then, an imaginary value (24) of some kinematical quantum variables has a big advantage: it allows us to formulate the quantum constrained system without violating uncertainty relations. For an unconstrained system, we have the generalized uncertainty relation

$$G^{qq}G^{pp} - (G^{qp})^2 \geq \frac{1}{4}\hbar^2. \quad (25)$$

This relation, which is important for an analysis of coherent states, would be violated had we worked with real quantum constraints $G^{qq} \approx 0 \approx G^{qp}$ instead of $(C^{(2)}, C_p^{(1)})$. Again, this is not problematic because the uncertainty relation is formulated with respect to the kinematical inner product, which may change. Still, the uncertainty relations are useful to construct coherent states and it is often helpful to have them at ones disposal. They can be formulated without using self-adjointness, but this would require one to treat \hat{q} , \hat{p} as well as \hat{q}^\dagger and \hat{p}^\dagger as independent such that their commutators (needed on the right hand side of an uncertainty relation) are unknown. The imaginary value of G^{qp} obtained with our definition of the quantum constraints, on the other hand, allows us to implement the constraints in a way respecting the standard uncertainty relation: $-(G^{qp})^2 = \frac{1}{4}\hbar^2$ from (24) saturates the relation.

4.2 Discrete momentum as constraint: $\hat{C} = \hat{p}$ on a circle

We now assume classical phase space variables $\phi \in S^1$ with momentum p . This requires a non-canonical basic algebra generated by the operators \hat{p} , $\widehat{\sin \phi}$ and $\widehat{\cos \phi}$ with

$$[\widehat{\sin \phi}, \hat{p}] = \widehat{\cos \phi} \quad , \quad [\widehat{\cos \phi}, \hat{p}] = -\widehat{\sin \phi} . \quad (26)$$

This example can also be seen as a model for isotropic loop quantum cosmology and gravity [23, 24, 25].

The constraint operator $\hat{C} = \hat{p}$ implies the presence of quantum constraints $C_Q = p$ as well as $C_p^{(n-1)} \approx G^{p^n}$. This is not sufficient to remove all quantum variables by constraints or gauge, and we need to include quantum constraints referring to ϕ . Unlike in Sec. 4.1, we cannot take $f = \phi$ because there is no operator for ϕ . If we choose $C_{\sin \phi}^{(n)}$ as starting point, the requirement of a closed set of constraints generates $C_{1 \cdot [p, \sin \phi]}^{(n)} = -C_{\cos \phi}^{(n)}$. Taken together, those constraints generate $C_{\sin \phi [p, \cos \phi]}^{(n)} = C_{\sin^2 \phi}^{(n)}$, $C_{\sin \phi [p, \sin \phi]}^{(n)} = -C_{\sin \phi \cos \phi}^{(n)}$ and $C_{\cos \phi [p, \sin \phi]}^{(n)} = -C_{\cos^2 \phi}^{(n)}$, i.e. all quantum constraints $C_{f(\phi)}^{(n)}$ with a function f depending on ϕ polynomially of second degree through $\sin \phi$ and $\cos \phi$. Iterating the procedure results in a closed set of constraints p , G^{p^n} and $C_{P(\sin \phi, \cos \phi)}^{(n)}$ with arbitrary polynomials $P(x, y)$.

In this case, we have independent uncertainty relations for each pair of self-adjoint operators. Relevant for consistency with the constraints is the relation

$$G^{pp} G^{\cos \phi \cos \phi} - (G^{p \cos \phi})^2 \geq \frac{1}{4} \hbar^2 \langle \widehat{\sin \phi} \rangle^2$$

and its obvious analog exchanging $\cos \phi$ and $\sin \phi$. Also here, one can see as before that the imaginary part of $G^{p \cos \phi} = C_{\cos \phi}^{(1)} - p \cos \phi + \frac{1}{2} i \hbar \sin \phi \approx \frac{1}{2} i \hbar \sin \phi$ allows one to respect the uncertainty relation even though $G^{pp} \approx 0$.

Note that this is similar to the previous example, although now zero being in the discrete spectrum of \hat{p} would allow one to use a physical Hilbert space as a subspace of the kinematical one whose reality conditions could thus be preserved. If this is done, $G^{p \cos \phi}$ must be real even kinematically because the kinematical inner product determines the physical one just by restriction. The uncertainty relation in this example turns out to be respected automatically, even for real kinematical quantum variables, because the algebra (26) of operators implies that $\langle \widehat{\sin \phi} \rangle = \langle [\widehat{\cos \phi}, \hat{p}] \rangle = 0$ in physical states. Moreover, $G^{p \cos \phi} \approx \frac{1}{2} i \hbar \sin \phi \approx 0$ turns out to be real on the constraint surface, after all.

Alternatively, if one knows that the constraint is represented as a self-adjoint operator with zero in the discrete part of its spectrum, the same relations can be recovered by appealing directly to the existence of creation and annihilation operators which map zero eigenstates of the constraint to other states in the kinematical Hilbert space. For these operators to exist, the physical Hilbert space must indeed be a subspace of the kinematical Hilbert space (given by zero eigenstates of the constraint operator and the inner product on those states) such that this argument explicitly refers to the discrete spectrum case only. Using this information about the quantum representation makes it possible to do the

reduction of effective constraints without introducing complex-valued kinematical quantum variables. Indeed, in our case $\hat{a}^\dagger = \widehat{\cos \phi} + i\widehat{\sin \phi}$ and $\hat{a} = \widehat{\cos \phi} - i\widehat{\sin \phi}$, respectively, raise and lower the discrete eigenvalues of \hat{p} represented on the Hilbert space $L^2(S^1, d\phi)$. For any eigenstate of \hat{p} , then, $\langle \hat{a}^\dagger \rangle = \langle \widehat{\cos \phi} \rangle + i\langle \widehat{\sin \phi} \rangle = 0$ and $\langle \hat{a} \rangle = \langle \widehat{\cos \phi} \rangle - i\langle \widehat{\sin \phi} \rangle = 0$. Thus, we again derive that the right hand side of uncertainty relations vanishes in physical states, making real-valued kinematical quantum variables consistent. Moreover, this example shows that for a constraint with zero in the discrete part of its spectrum, additional constraints follow which can be used to eliminate variables which in the general effective treatment appear as gauge. In fact, all moments involving $\sin \phi$ or $\cos \phi$ are constrained to vanish if $\langle \hat{a}^n \rangle = 0 = \langle (\hat{a}^\dagger)^m \rangle$ is used for physical states. In this case, no gauge flow is necessary to factor out these moments, but in contrast to the gauge flow itself this can only be seen based on representation properties.

Using complex valued kinematical quantum variables turns out to be more general and applicable to constraints with zero in the discrete or continuous spectrum. For systems with zero in the discrete spectrum, this can be avoided but requires one to refer explicitly to properties of the quantum representation or the operator algebra.

4.3 Two component system with constraint: $\hat{C} = \hat{p}_1 - \hat{p}$

As an example which can be interpreted as a parameterized version of an unconstrained system, we consider a system with a 4-dimensional phase space and phase space coordinates $(q, p; q_1, p_1)$. The system is governed by a linear constraint

$$C_Q = p_1 - p . \quad (27)$$

The classical constraint can, of course, be transformed canonically to a constraint which is identical to one of the phase space coordinates since $(\frac{1}{2}(q_1 - q), C; \frac{1}{2}(q_1 + q), p_1 + p)$ forms a system of canonical coordinates and momenta containing $C = p_1 - p$. Moreover, the transformation is linear and can easily be taken over to the quantum level as a unitary transformation. The orders of moments do not mix under such a linear transformation, and thus the arguments put forward in Sec. 4.1 can directly be used to conclude that the system discussed here is consistent and complete. Nevertheless, it is instructive to look at details of the procedure without doing such a transformation, which will serve as a guide for more complicated cases.

Expectation values satisfy the classical gauge transformations

$$-\dot{q} = 1 = \dot{q}_1 \quad , \quad \dot{p} = 0 = \dot{p}_1 . \quad (28)$$

At this point, we recall that there are no reality or positivity conditions for the kinematical quantum variables (4) as they appear before solving any constraints. Their gauge transformations are

$$\dot{G}_{c,d}^{a,b} = 0 , \quad (29)$$

where

$$G_{c,d}^{a,b} = \langle (\hat{p} - p)^a (\hat{q} - q)^b (\hat{p}_1 - p_1)^c (\hat{q}_1 - q_1)^d \rangle_{\text{Weyl}} . \quad (30)$$

Even though these variables remain constant, as do those of the deparameterized system, here we have additional moments compared to an unconstrained canonical pair: solving the constraints has to eliminate all quantum variables with respect to one canonical pair, but also cross-correlations to the unconstrained pair. These cannot all be set to zero simultaneously due to the uncertainty relations — but they may be chosen to satisfy minimal uncertainty.

4.3.1 Constraints

In addition to gauge transformations (28) and (29) generated by the principal quantum constraint $C_Q = C^{(1)}$, the system is subject to further constraints and their gauge transformations. As explained above, the quantum constraints have to form a complete, first class set. Such a set is given by

$$\begin{aligned}
C^{(n)} &= \sum_{m=0}^n \sum_{k=0}^m \sum_{\ell=0}^{n-m} \binom{n}{m} \binom{m}{k} \binom{n-m}{\ell} (-1)^{n-m} p_1^k p^\ell G_{m-k,0}^{n-m-\ell,0} \\
C_q^{(n)} &= \sum_{m=0}^n \sum_{k=0}^m \sum_{\ell=0}^{n-m} \binom{n}{m} \binom{m}{k} \binom{n-m}{\ell} (-1)^{n-m} p_1^k p^\ell \left(G_{m-k,0}^{n-m-\ell,1} - \frac{i\hbar}{2} (n-m-\ell) G_{m-k,0}^{n-m-\ell-1,0} \right) \\
C_p^{(n)} &= \sum_{m=0}^n \sum_{k=0}^m \sum_{\ell=0}^{n-m} \binom{n}{m} \binom{m}{k} \binom{n-m}{\ell} (-1)^{n-m} p_1^k p^\ell \left(p G_{m-k,0}^{n-m-\ell,0} + G_{m-k,0}^{n-m-\ell+1,0} \right) \\
C_{p_1}^{(n)} &= \sum_{m=0}^n \sum_{k=0}^m \sum_{\ell=0}^{n-m} \binom{n}{m} \binom{m}{k} \binom{n-m}{\ell} (-1)^{n-m} p_1^k p^\ell \left(p_t G_{m-k,0}^{n-m-\ell,0} + G_{m-k+1,0}^{n-m-\ell,0} \right) \\
C_{q_1}^{(n)} &= \sum_{m=0}^n \sum_{k=0}^m \sum_{\ell=0}^{n-m} \binom{n}{m} \binom{m}{k} \binom{n-m}{\ell} (-1)^{n-m} p_1^k p^\ell \left(G_{m-k,1}^{n-m-\ell,0} + \frac{i\hbar}{2} (m-k) G_{m-k-1,0}^{n-m-\ell,0} \right).
\end{aligned}$$

These constraints are accompanied by analogous expressions involving polynomial factors of the basic operators, which we will not be using to the orders considered here. We thus solve our constraints as given to the required orders and determine the gauge orbits they generate.

At this point, a further choice arises: we need to determine which variables we want to solve in terms of others which are to be kept free. This is related to the choice of time in a deparametrization procedure. Here, we view q_1 as the time variable which is demoted from a physical variable to the status of an evolution parameter, and thus $H = p$ will be the Hamiltonian generating evolution in this time. Notice that time is chosen after quantization when dealing with effective constraints. (For our linear constraint, of course, the roles of the two canonical pairs can be exchanged, with q playing the role of time.)

Classically, it is then straightforward to solve the constraint and discuss gauge, and the same applies to expectation values in the quantum theory. The discussion of quantum variables is, however, non-trivial and is therefore presented here in some detail for second order moments. Having made a choice of time, a complete deparametrization requires that

all quantum variables of the form $G_{a_2, b_2}^{a_1, b_1}$ with $a_2 \neq 0$ or $b_2 \neq 0$ be completely constrained or removed by gauge. Only quantum variables $G_{0,0}^{a,b}$ are allowed to remain free, and must do so without any further restrictions. To second order, the deparametrized system has $2+3=5$ variables; the parametrized theory has $4+10=14$. We begin by eliminating quantum variables in favor of the variables associated with the canonical pair (q_1, p_1) only. From the fact that, on the one hand, $G_{p_1 p_1}$, $G_{p_1 q_1}$ and $G_{q_1 q_1}$ should satisfy the uncertainty relations and thus cannot all vanish but, on the other hand, are not present in the unconstrained system, we expect at least one of them to be removed by gauge.

At second order,⁷ i.e. keeping only second order moments as well as terms linear in \hbar , the constraints form a closed and complete system given by

$$\begin{aligned} C^{(n)}|_{N=2} &= c_n + d_n (G^{pp} + G_{p_1 p_1} - 2G_{p_1}^p) \\ C_p^{(n)}|_{N=2} &= a_n \left(G^{pq} - G_{p_1}^p - \frac{i\hbar}{2} \right) + b_n (G^{pp} - 2G_{p_1}^p + G_{p_1 p_1}) \\ C_q^{(n)}|_{N=2} &= a_n (G^{pp} - G_{p_1}^p) \\ C_{p_1}^{(n)}|_{N=2} &= a_n (G_{p_1}^p - G_{p_1 p_1}) \\ C_{q_1}^{(n)}|_{N=2} &= a_n \left(G_{q_1}^p - G_{p_1 q_1} - \frac{i\hbar}{2} \right) + c_n (G_{p_1 p_1} - 2G_{p_1}^p + 2c_n G^{pp}) , \end{aligned}$$

where

$$\begin{aligned} a_n &= a_n(p_1, q) \equiv -n(C^{(1)})^{n-1} , \quad b_n = b_n(p_1, q) \equiv \frac{i\hbar}{2} n(n-1)(n-2)(C^{(1)})^{n-3} \\ c_n &= c_n(p_1, q) \equiv (C^{(1)})^n , \quad d_n = d_n(p_1, q) \equiv \frac{n}{2}(n-1)(C^{(1)})^{n-2} , \end{aligned}$$

and $C^{(1)} = p_1 - p$ is the linear constraint which in this case is identical with the classical constraint.

Due to the fact that the prefactors in the constraint equations contain $C^{(1)}$, we find non-trivial constraints only when the exponent of $C^{(1)}$ vanishes. This happens for a_1 , b_3 and d_2 , while c_n vanishes for all n . For higher n no additional constraints arise. Constraints arising for $n=2, 3$ turn out to be linear combinations of the constraints arising for $n=1$. Therefore we find for the second order system only five independent constraints: $C^{(1)}|_{N=2} = p_1 - p$ and

$$\begin{aligned} C_q^{(1)}|_{N=2} &= -\frac{i\hbar}{2} - G^{qp} + G_{p_1}^q , \quad C_p^{(1)}|_{N=2} = G_{p_1}^p - G^{pp} \\ C_{p_1}^{(1)}|_{N=2} &= G_{p_1 p_1} - G_{p_1}^p , \quad C_{q_1}^{(1)}|_{N=2} = \frac{i\hbar}{2} - G_{q_1}^p + G_{q_1 p_1} . \end{aligned}$$

From these equations it is already obvious that four second order moments referring to q_1 or p_1 can be eliminated through the use of constraints. In addition to $p_1 = p$ for expectation

⁷The moment expansion is formalized in Sec. 6.1.

values, these are

$$G_{p_1}^q \approx \frac{1}{2}i\hbar + G^{qp} \quad , \quad G_{p_1}^p \approx G^{pp} \quad , \quad G_{p_1 p_1} \approx G_{p_1}^p \approx G^{pp} \quad (31)$$

as well as

$$G_{q_1}^p \approx \frac{1}{2}i\hbar + G_{q_1 p_1} \quad (32)$$

which is not yet completely expressed in terms of moments only of (q, p) . The remaining moments of (q_1, p_1) are not constrained at all, and thus must be eliminated by gauge transformations. To summarize, three expectation values are left unconstrained, one of which should be unphysical; six second-order variables are unconstrained, three of which should be unphysical. Notice that there is no contradiction to the fact that we have four weakly commuting (and independent) constraints but expect only three variables to be removed by gauge. These are constraints on the space of second order moments, which, in this truncation, as noted before do not have a non-degenerate Poisson bracket (although the space of all moments has a non-degenerate symplectic structure). Weak commutation then does not imply first class nature in the traditional sense (see e.g. [21]), and four weakly commuting constraints may declare less than four variables as gauge. While the constraints as functionals are independent, their gauge flows may be linearly dependent.

4.3.2 Observables

To explicitly account for the unphysical degrees of freedom, we consider the gauge transformations generated by the constraints. The quantum constraint $p_1 - p \approx 0$ produces a flow on the expectation values only, which agrees with the classical flow (28). The second-order constraints, produce no (independent)⁸ flow on the expectation values.

Also G^{pp} is gauge invariant. For the five remaining free second-order variables, $G_{p_1}^p - G^{pp} \approx 0$ generates a flow (on the constraint surface):

$$\begin{aligned} \delta G^{qp} &= G_{p_1}^p - 2G^{pp} \approx -G^{pp} \\ \delta G^{qq} &= 2G_{p_1}^q - 4G^{qp} \approx i\hbar - 2G^{qp} \\ \delta G_{q_1 p_1} &= G_{p_1}^p \approx G^{pp} \\ \delta G_{q_1}^q &= G_{q_1 p_1} + G^{qp} - 2G_{q_1}^p \approx G^{qp} - G_{q_1 p_1} - i\hbar \\ \delta G_{q_1 q_1} &= G_{q_1}^p \approx i\hbar + 2G_{q_1 p_1} \end{aligned} \quad (33)$$

$G_{p_1}^p - G^{pp} \approx 0$ gives:

$$\begin{aligned} \delta G^{qp} &\approx G^{pp} \quad , \quad \delta G^{qq} \approx i\hbar + 2G^{qp} \quad , \quad \delta G_{q_1 p_1} \approx -G^{pp} \\ \delta G_{q_1}^q &\approx G_{q_1 p_1} - G^{qp} - i\hbar \quad , \quad \delta G_{q_1 q_1} \approx i\hbar - 2G_{q_1 p_1} \end{aligned} \quad (34)$$

⁸The parts of the second-order constraints proportional to $C^{(1)}$ that have been discarded can also be ignored when computing the flows generated on the constraint surface, as the missing contributions are proportional to the gauge flow associated with $C^{(1)}$. This is true in general, and extends to higher orders.

$\frac{1}{2}i\hbar + G^{qp} - G_{p_1}^q \approx 0$ gives:

$$\begin{aligned} \delta G^{qp} &\approx \frac{1}{2}i\hbar + G^{qp} \quad , \quad \delta G^{qq} \approx 2G^{qq} \quad , \quad \delta G_{q_1 p_1} \approx -\frac{1}{2}i\hbar - G^{qp} \\ \delta G_{q_1}^q &\approx G_{q_1}^q - G^{qq} \quad , \quad \delta G_{q_1 q_1} \approx -2G_{q_1}^q \end{aligned} \quad (35)$$

$\frac{1}{2}i\hbar - G_{q_1}^p + G_{q_1 p_1} \approx 0$ gives:

$$\begin{aligned} \delta G^{qp} &\approx -\frac{1}{2}i\hbar - G_{q_1 p_1} \quad , \quad \delta G^{qq} \approx -2G_{q_1}^q \quad , \quad \delta G_{q_1 p_1} \approx \frac{1}{2}i\hbar + G_{q_1 p_1} \\ \delta G_{q_1}^q &\approx G_{q_1}^q - G_{q_1 q_1} \quad , \quad \delta G_{q_1 q_1} \approx 2G_{q_1 q_1} \end{aligned} \quad (36)$$

All of the gauge flows obey

$$\delta G^{qp} = -\delta G_{q_1 p_1} \quad , \quad \delta G_{q_1}^q = -\frac{1}{2}(\delta G^{qq} + \delta G_{q_1 q_1}) \quad . \quad (37)$$

Thus, in addition to $A_1 := G^{pp}$ we can identify the observables $A_2 := G^{qq} + 2G_{q_1}^q + G_{q_1 q_1}$ and $A_3 := G^{qp} + G_{q_1 p_1}$. They satisfy the algebra $\{A_1, A_3\} = -2A_1$, $\{A_1, A_2\} \approx -4(A_3 + \frac{1}{2}i\hbar)$, $\{A_2, A_3\} = 2A_2$ on the constraint surface which, except for the imaginary term, agrees with the Poisson algebra expected for unconstrained quantum variables of second order. The imaginary term can easily be absorbed into the definition of A_3 , which leads us to the physical quantum variables

$$\mathcal{G}^{qq} := G^{qq} + 2G_{q_1}^q + G_{q_1 q_1} \quad , \quad \mathcal{G}^{pp} := G^{pp} \quad , \quad \mathcal{G}^{qp} := G^{qp} + G_{q_1 p_1} + \frac{1}{2}i\hbar \quad . \quad (38)$$

They commute with all the constraints and satisfy the standard algebra for second order moments, thus providing the correct representation. To implement the physical inner product, we simply demand that all the physical quantum variables be real. This means that $G^{qp} + G_{q_1 p_1}$ must have the imaginary part $-\frac{1}{2}i\hbar$ which is possible for kinematical quantum variables.

4.3.3 Gauge fixing

In fact, one can choose a gauge where all physical quantum variables agree with the kinematical quantum variables of the pair (q, p) , and kinematical quantum variables of the pair (q_1, p_1) satisfy $G_{p_1 p_1} = 0$ and $G_{q_1 p_1} = -\frac{1}{2}i\hbar$. This choice violates kinematical reality conditions, but it ensures physical reality and preserves the kinematical uncertainty relation even though one fluctuation vanishes.

Other gauge choices are possible since only $G^{qp} + G_{q_1 p_1}$ is required to have imaginary part $-\frac{1}{2}i\hbar$ for real \mathcal{G}^{qp} , which can be distributed in different ways between the two moments. Thus, there are different choices of the kinematical reality conditions. Such gauge choices may be related to some of the freedom contained in choosing the kinematical Hilbert space which would similarly affect the reality of kinematical quantum variables.

The algebra of the physical variables can be recovered without the knowledge of their explicit form as observables, by completely fixing the gauge degrees of freedom and using

the Dirac bracket to find the Poisson structure on the remaining free parameters. We introduce gauge conditions $\phi_i = 0$ which together with the second order constraints define a symplectic subspace Σ_ϕ of the space of second order quantum variables. Our conditions should fix the gauge freedom entirely — which means that the flow due to any remaining first class constraints should vanish on Σ_ϕ . (We recall that the space of second order moments does not form a symplectic subspace of the space of all moments, but it does define a Poisson manifold. In such a situation, not all first class constraints need to be gauge-fixed to obtain a symplectic gauge-fixing surface.) In order to ensure that the conditions put no restrictions on the physical degrees of freedom, we demand that no non-trivial function of the gauge conditions be itself gauge invariant.

The simple gauge discussed above corresponds to $\phi_4 = G_{p_1 q_1} + \frac{1}{2}i\hbar = 0$, $\phi_5 = G_{q_1 q_1} = 0$ and $\phi_6 = G_{q_1}^q = 0$. Under these conditions $C_{q_1}^{(1)}$ remains first class but has a vanishing flow (36) on the surface Σ_ϕ . The other second order constraints now form a second class system when combined with the gauge conditions. The combination of constraints and gauge fixing conditions eliminates all second order variables except for G^{pp} , G^{qq} and G^{qp} , which therefore parameterize Σ_ϕ . Labeling $\phi_1 = C_p^{(1)}$, $\phi_2 = C_q^{(1)}$, $\phi_3 = C_{p_1}^{(1)}$, the commutator matrix $\Delta_{ij} := \{\phi_i, \phi_j\}$ on Σ_ϕ ,

$$\Delta|_{\Sigma_\phi} = \begin{pmatrix} 0 & 0 & 0 & -G^{pp} & 0 & \frac{1}{2}i\hbar - G^{qp} \\ 0 & 0 & 0 & \frac{1}{2}i\hbar + G^{qp} & 0 & G^{qq} \\ 0 & 0 & 0 & G^{qq} & -2i\hbar & \frac{1}{2}i\hbar + G^{qp} \\ G^{pp} & -\frac{1}{2}i\hbar - G^{qp} & -G^{qq} & 0 & 0 & 0 \\ 0 & 0 & 2i\hbar & 0 & 0 & 0 \\ G^{qp} - \frac{1}{2}i\hbar & -G^{qq} & -\frac{1}{2}i\hbar - G^{qp} & 0 & 0 & 0 \end{pmatrix}$$

is invertible. The Dirac bracket $\{f, g\}_{\text{Dirac}} := \{f, g\} - \{f, \phi_i\} (\Delta^{-1})^{ij} \{\phi_j, g\}$ for a second class system of constraints can easily be computed for the remaining free parameters G^{qq} , G^{pp} and G^{qp} , recovering precisely the algebra satisfied by the physical quantum variables (38). Thus, fixing the gauge freedom entirely, we recover the physical Poisson algebra. In a general situation, where finding the explicit form of observables is more difficult, this alternative method of obtaining their Poisson algebra is easier to utilize.

5 Truncations

Linear constraints show that consistency and completeness are satisfied in our formulation of effective constraints. Locally, every constraint can be linearized by a canonical transformation, but global issues may be important especially in the quantum theory. Moreover, moments transform in complicated ways under general canonical transformations, mixing the orders of quantum variables. We will thus discuss non-linear examples to show the practicality of our procedures. Before doing so, we provide a more systematic analysis of the treatment of infinitely many constraints as they arise on the quantum phase space.

The above examples only considered quantum variables up to second order. A reduction of this form is always necessary if one intends to derive effective equations from a

constrained system. For practical purposes, infinite dimensional systems have to be reduced to a certain finite order of quantum variables so that one can actually retrieve some information from the system. There are two possibilities to do this: an approximate solution scheme order by order, or a sharp truncation. It is then necessary to check whether the system of constraints can still be formulated in a consistent way after such a reduction has been carried out. A priori one cannot assume, for instance, that a sharply truncated system of constraints has any non-trivial solution at all. It may turn out that all degrees of freedom are removed by the truncated constraints. Also it is not clear how many (truncated) constraints have to be taken into account at a certain order of the truncation. In this section, we first consider a linear example and show that it can consistently be truncated. We then turn to the more elaborate and more physical example of the parametrized free, non-relativistic particle. Here, sharp truncations turn out to be inconsistent. While this makes sharp truncations unreliable as a general tool, it is instructive to go through examples where they are inconsistent. The following section will then be devoted to consistent approximations without a sharp truncation.

5.1 Truncated system of constraints for $\hat{C} = \hat{q}$

The system as in Sec. 4.1 is governed by a constraint $C_{\text{class}} = q$ which on the quantum level entails the constraint operator $\hat{C} = \hat{q}$. (We explicitly denote the classical constraint as C_{class} because by our general rule we reserve the letter C for the expectation value $\langle \hat{C} \rangle$.) This implies the following constraints on the quantum phase space:

$$\begin{aligned} C^{(n)} &= \langle \hat{C}^n \rangle = C_{\text{class}}^n + \sum_{j=0}^{n-1} \binom{n-1}{j} C_{\text{class}}^j G_{0,n-j} \quad , \quad C_q^{(n)} = \langle \hat{q} \hat{C}^n \rangle = C^{(n+1)} \\ C_p^{(n)} &= \langle \hat{p} \hat{C}^n \rangle = p C_{\text{class}}^n + p \sum_{j=0}^{n-1} \binom{n}{j} C_{\text{class}}^j G_{0,n-j} + \sum_{j=0}^{n-1} \binom{n}{j} \frac{C_{\text{class}}^j}{a_{n-j}} \left(G_{1,n+1} - i\hbar \frac{(n-j)^2}{(n-j+1)} G_{0,n-j-1} \right) \end{aligned}$$

where a_{n-j} are constant coefficients. These are accompanied by similar expressions of higher polynomial constraints, i.e. $C_{p^m}^{(n)}$ which are more lengthy in explicit form due to the reordering involved in quantum variables.

The lowest power constraint yields $C^{(1)} = C_{\text{class}} \approx 0$. Inserting this, the higher power constraints reduce to

$$\begin{aligned} C^{(n)} &\approx G_{0,n} \quad , \quad C_q^{(n)} \approx G_{0,n+1} \\ C_p^{(n)} &\approx p G_{0,n} + \frac{1}{a_n} \left(G_{1,n} - i\hbar \frac{n^2}{(n+1)^2} G_{0,n-1} \right) . \end{aligned}$$

Now, a sharp truncation at N^{th} order implies setting $G_{a,b} = 0$ for all $a+b > N$. As non-trivial constraints remain

$$C^{(n)}|_N \approx G_{0,n} \quad \text{for all } n \leq N$$

$$\begin{aligned}
C_p^{(n)}|_N &\approx pG_{0,n} + \frac{1}{a_n} \left(G_{1,n} - i\hbar \frac{n^2}{(n+1)^2} G_{0,n-1} \right) \quad \text{for all } n \leq N-1 \\
C_p^{(N)}|_N &\approx pG_{0,N} + \frac{1}{a_N} \left(-i\hbar \frac{N^2}{(N+1)^2} G_{0,N-1} \right) \quad \text{for } n = N.
\end{aligned}$$

Solving the quantum constraints $C^{(n)} \approx 0$ and inserting the solutions into the constraints $C_p^{(n)}$, yields

$$\begin{aligned}
C_p^{(n)}|_N &\approx \frac{1}{a_n} G_{1,n} \quad \text{for all } n \leq N-1 \\
C_p^{(n)}|_N &\approx 0 \quad \text{for all } n \geq N.
\end{aligned}$$

Thus we find that for the truncated system, $G_{0,n}$ are eliminated through the constraints $C^{(n)} = 0$, whereas the quantum variables $G_{1,n}$ are eliminated through $C_p^{(n)} = 0$. Higher polynomial constraints fix all remaining moments except $G_{n,0}$: They can be expanded as

$$\begin{aligned}
C_{p^k}^{(n)} &= \sum_{i=0}^k \sum_{j=0}^n \binom{k}{i} \binom{n}{j} p^i C_{\text{class}}^j \langle (\hat{p} - p)^{k-i} (\hat{q} - q)^{n-j} \rangle \\
&\approx \sum_{i=0}^k \binom{k}{i} p^i \langle (\hat{p} - p)^{k-i} (\hat{q} - q)^n \rangle = \frac{G_{k,n}}{b_{k,n}} + \dots
\end{aligned}$$

with some coefficients $b_{k,n}$ and where moments of lower order in p are not written explicitly because they can be determined from constraints of smaller k . Due to the constraint $C^{(1)} = C_{\text{class}} \approx 0$, moreover, expectation values are restricted to the classical constraint hypersurface. No further restrictions on these degrees of freedom arise and also the gauge flows act in the proper way. In particular, all remaining unconstrained $G_{n,0}$ become pure gauge. (This again confirms considerations in Sec. 3.1.2 because the gauge flow of $C_{q^m}^{(n)} = C^{(n+m)}$ is sufficient to remove all gauge without making use of $C_{p^m}^{(n)}$ with $m \neq 0$, where operators not commuting with the constraint would occur.) The system can thus be truncated consistently. For a truncation at N^{th} order of a linear classical constraint, constraints up to order N have to be taken into account.

However, the linear case is quite special because we only had to truncate the system of constraints, but not individual constraints: any effective constraint contains quantum variables of only one fixed order. Referring back to section 3.1.2, when \hat{C} is linear, we can impose all of the constraints and remove all of the gauge degrees of freedom in variables up to a given order without invoking higher-order constraints. This is accomplished by treating higher-order constraints as imposing conditions on higher-order quantum variables (possibly in terms of the lower-order unconstrained variables) and noting that using Eq. (14) there is no need to refer to constraints of order above $F^{a_1, a_2, \dots, a_{2N}; b, 0}$ itself in order to demonstrate that it is a pure-gauge variable. The gauge-invariant degrees of freedom that remain weakly commute with *all* constraints and not just the constraints up to the order considered; see Eq. (12). As a result, in the linear examples of Sec. 4, higher order

constraints do not affect the reduction of the degrees of freedom for orders below and so could be disregarded without making any approximations. For non-linear constraints, however, orders of moments mix and constraints relevant at low orders can contain moments of higher order. It is then more crucial to see how the higher moments could be disregarded consistently, as we will do in what follows.

5.2 Truncated system of constraints for the parametrized free non-relativistic particle

The motion of a free particle of mass M in one dimension is described on the phase space (p, q) . Through the introduction of an arbitrary time parameter t , time can be turned into an additional degree of freedom. The system is then formulated on the 4-dimensional phase space with coordinates $(t, p_t; q, p)$. The Hamiltonian constraint of the parametrized free non-relativistic particle is given by

$$C_{\text{class}} = p_t + \frac{p^2}{2M} , \quad (39)$$

which is constrained to vanish.

Promoting phase space variables to operators, Dirac constraint quantization yields the quantum constraint

$$\left(\hat{p}_t + \frac{\hat{p}^2}{2M} \right) \Psi = 0 . \quad (40)$$

In the Schrödinger representation, one arrives at an equation that is formally equivalent to the time-dependent Schrödinger equation⁹

$$i\hbar \frac{\partial \Psi(t, q)}{\partial t} = \frac{\hbar^2}{2M} \frac{\partial^2 \Psi(t, q)}{\partial q^2} . \quad (41)$$

As is well known, solutions to this equation are given by

$$\Psi(t, q) = \int dk A(k) e^{\frac{i}{\hbar} E(k)t + ikq} \quad (42)$$

where $E(k) = \frac{\hbar^2 k^2}{2M}$.

For the quantum variables we use, as before, the notation

$$G_{c,d}^{a,b} = \langle (\hat{p} - p)^a (\hat{q} - q)^b (\hat{p}_t - p_t)^c (\hat{t} - t)^d \rangle_{\text{Weyl}} . \quad (43)$$

In their general form, the set of constraints on the quantum phase space is given in the Appendix.

⁹In contrast to the ordinary, time-dependent Schrödinger equation, time is an operator in the equation obtained here and not an external parameter. This implies that the Hamiltonian which generates evolution in time, $\hat{\mathcal{H}}_{\text{phys}} = \frac{\hat{p}^2}{2M}$, has the same action on physical states as the momentum operator canonically conjugate to time. In contrast to the physical Hamiltonian, which is bounded below and positive semidefinite, the spectrum of the time momentum \hat{p}_t covers the entire real line. On physical solutions, however, only positive “frequencies” contribute.

5.2.1 Zeroth order truncation

Truncation of the system at zeroth order, i.e. setting all quantum variables to zero, yields $C^{(n)}|_{N=0} = C_{\text{class}}^n$ together with

$$C_q^{(n)}|_{N=0} = qC_{\text{class}}^n + \frac{i\hbar}{2}n\frac{p}{m}C_{\text{class}}^{n-1} \quad , \quad C_t^{(n)}|_{N=0} = tC_{\text{class}}^n + \frac{i\hbar}{2}nC_{\text{class}}^{n-1}$$

as the required constraints. This truncation is *not* consistent. Inserting the condition $C_{\text{class}} = 0$ from the first in the remaining constraints, especially in $C_t^{(1)}|_{N=0} = tC_{\text{class}} + \frac{1}{2}i\hbar$, results in $\frac{i\hbar}{2} = 0$. The reason may seem clear: A truncation at zeroth order can be understood as neglecting all quantum properties of the system. But this is not possible for a free particle. There is no solution in which e.g., both, spread in p and q would be negligible throughout the particle's evolution. There is no wave-packet which would remain tightly peaked throughout the evolution and a description in terms of expectation values alone seems insufficient in this case.

5.2.2 Second order truncation

But even if one takes into account the second order quantum variables, spreads and fluctuations, an inconsistent system results. The expanded constraints can also be found in the appendix, which we now sharply truncate at second order in moments. From $C^{(n)}$ only three non-trivial constraints follow

$$\begin{aligned} C^{(1)} &= C_{\text{class}} + \frac{1}{2M}G_{0,0}^{2,0} \\ C^{(2)}|_{N=2} &= C_{\text{class}}^2 - (6C_{\text{class}} - 4p_t)G_{0,0}^{2,0} + \frac{4p}{2M}G_{1,0}^{1,0} + G_{2,0}^{0,0} \\ C^{(3)}|_{N=2} &= C_{\text{class}}^3 \quad , \end{aligned}$$

upon inserting the constraints successively. Thus for an $N = 2$ order truncation, at $n = 3$, the classical constraint is recovered and must vanish for the truncated system. Then, $C^{(1)} \approx 0$ yields $G_{0,0}^{2,0} \approx 0$ which is too strong for a consistent reduction since one expects the fluctuation G^{pp} to be freely specifiable. It has to remain a physical degree of freedom after solving the constraints, for otherwise no general wave packet as in (42) can be posed as an initial condition of the free particle. In the sharp truncation, it turns out, there are too many constraints which overdetermine the system. Especially the constraint $C^{(3)}$, when truncated to second order moments, reduces to the classical constraint C_{class}^3 , which then immediately implies $G^{pp} = 0$ due to $C^{(1)}$.

This observation points to a resolution of the inconsistency: While $C^{(1)}$ is already of second order even without a truncation, $C^{(3)}$ contains higher order moments. The truncation is then inconsistent in that we are ignoring higher orders next to an expression which we then constrain to be zero. For unconstrained moments, this would be consistent; but it is not if some of the moments are constrained to vanish. Thus, a more careful approximation scheme must be used where we do not truncate sharply but ignore higher

moments only when they appear together with lower moments *not constrained to vanish*. In such a scheme, as discussed in the following section, $C^{(3)}$ would pose a constraint on the higher moments in terms of $C_{\text{class}} \approx -G^{pp}/2M$, but would not require C_{class} or G^{pp} to vanish.

6 Consistent approximations

Through the iteration described in Sec. 3.1, the polynomial constraints of Sec. 3.1.2 or the generating function of Sec. 3.2 one arrives at an infinite number of constraints imposed on an infinite number of quantum variables. The linear systems have already demonstrated consistency and completeness of the whole system, but for practical purposes the infinite number of constraints and variables is to be reduced. We have seen in the preceding section that sharp truncations are in general inconsistent and that more careful approximation schemes are required. Depending on the specific reduction, it is neither obvious that the effective constraints are consistent in that they allow solutions for expectation values and moments at all, nor is it guaranteed that the constraints at hand do actually eliminate all unphysical degrees of freedom. For each classical canonical pair which is removed by imposing the constraints, all the corresponding moments as well as cross-moments with the unconstrained canonical variables should be removed. Classically, as well as in our quantum phase space formulation, the elimination of unphysical degrees of freedom is a twofold process: The constraints can either restrict unphysical degrees of freedom to specific functions of the physical degrees of freedom, or unphysical degrees of freedom can be turned into mere gauge degrees of freedom under the transformations generated by the constraints and then gauge fixed if desired.

In the following, we will first demonstrate by way of a non-trivial example, rather than referring to linearization, that the constraints as formulated in Sec. 3.1 are consistent, before turning to the elimination of the unphysical degrees of freedom. Our specific example is again the parametrized free non-relativistic particle, but the general considerations of Sec. 6.1 hold for any parameterized non-relativistic system.

We use the variables and constraints as they have been determined in Sec. 5.2. This establishes a hierarchy of the constraints, suggesting to solve $C^{(n)}$ first, then $C_q^{(n)}$, $C_t^{(n)}$, $C_{p_t}^{(n)}$ and $C_p^{(n)}$, and the remaining constraints (66)–(69) first for $k = 1$, then $k = 2$ etc. Note that for each k in (66)–(69) the $r = k$ term is the only contribution of a form not appearing at lower orders. The terms occurring in the r -sum are linear combinations of the constraints (66)–(69) for $k' < k$. Thus apart from the $r = k$ term all other terms vanish if the lower k constraints are satisfied.

It is important to notice that the structure of the constraints is such that on the constraint hypersurface $C^{(n)}$, $C_{qp^k}^{(n)}$, $C_q^{(n)}$, $C_{tp^k}^{(n)}$ and $C_t^{(n)}$ contain as lowest order terms expectation values, whereas $C_{pp^k}^{(n)}$, $C_p^{(n)}$, $C_{p_tp^k}^{(n)}$ and $C_{p_t}^{(n)}$ have second order moments as lowest contribution. The highest order moments occurring in $C^{(n)}$ are of order $2n$, $2n + 1$ for $C_q^{(n)}$, $C_t^{(n)}$, $C_p^{(n)}$ and $C_{p_t}^{(n)}$ and $2n + 1 + k$ in $C_{qp^k}^{(n)}$, $C_{tp^k}^{(n)}$, $C_{pp^k}^{(n)}$ and $C_{p_tp^k}^{(n)}$.

The structure of (66)–(69) implies that the lowest contributing order in the j - and ℓ -sums (on the constraint hypersurface) is $j + \ell + k \pm 1$ and rises with k . Consequently, there exists a maximal k up to which constraints have to be studied if only moments up to a certain order are taken into account. We check the consistency of the constraints order by order in the moments. This means that we first have to verify that one can actually solve the constraints for the expectation values. This analysis will then be displayed explicitly for second and third order moments.

6.1 General procedure and moment expansion

To verify consistency up to a certain order, one can exploit the fact that up to a fixed order N of the moments only a finite number of constraints have to be taken into account. This can be seen from the following argument: In the j - ℓ -summation, the relevant moments occur for $j + \ell \pm 1 \leq N$. From this condition, a number of pairs (j, ℓ) result for which the sums occurring in (64)–(69) can be evaluated. There remain sums over m containing p_t , which should be eliminated if we choose t as internal time to make contact with the quantum theory of the deparameterized system. (Our consistent approximation procedure, however, is more general and does not require the choice of an internal time.) We can achieve this by rewriting these as terms of the form $n(n-1) \cdots (n-g) C_{\text{class}}^{n-g-1}$ multiplied by powers of p and $2M$, where g is an integer depending on the values of j and ℓ . (See the examples in Eqs. (70)–(84).) This is achieved by eliminating p_t via¹⁰ $C^{(1)} = C_Q \approx 0$ and illustrates the central role played by the principal quantum constraint C_Q . For a fixed order N of moments, there is a factor of lowest and one of highest power of C_{class} . In $C^{(n)}$, e.g., the highest power is given for $j = 0, \ell = 0$ (with $m = n$) and is simply C_{class}^n , whereas the lowest power is given for $\ell = 0, j = N$ and is given by $n(n-1) \cdots (n-(N-1)) C_{\text{class}}^{n-N}$.¹¹

Since $C_{\text{class}} \approx -G_{0,0}^{2,0}/2M$, powers of second order moments ensue (or higher q -moments if there is a potential). Together with powers of \hbar in some of the terms, this must be compared with the orders of higher moments in order to approximate consistently. To formalize the required *moment expansions*, one can replace each moment $G_{c,d}^{a,b}$ by $\lambda^{a+b+c+d} G_{c,d}^{a,b}$ and expand in λ . This automatically guarantees that higher order moments appear at higher orders in the expansion, and that products of moments are of higher order than the moments themselves. Moreover, in order to leave the uncertainty relation unchanged, we have to replace \hbar by $\lambda^2 \hbar$, which ensures that it is of higher order, too, without performing a specific \hbar -expansion. After the λ -expansion has been performed, λ can be set equal to one to reproduce the original terms. (Assumptions of orders of moments behind this expansion scheme can easily be verified for Gaussian coherent states of the harmonic oscillator, where a moment $G^{a,b}$ is of order at least $\hbar^{(a+b)/2}$.)

One can now rewrite the sum over m for all those terms which produce factors with powers of C_{class} down to the lowest power occurring in front of the relevant moments. In

¹⁰In our example of the free particle, we have $C_Q = p_t + p^2/2M + G_{0,0}^{2,0}/2M$. If there is a potential, there will be further classical terms as well as quantum variables $G_{0,0}^{0,n}$.

¹¹This term arises of course as well for $\ell = N, j = 0, \ell = 1, j = N-1$, etc.

$C^{(n)}$ this would correspond to C_{class}^{n-N} . One can therefore rewrite the constraints in the form

$$C_{\text{class}}^n Y_1 + n C_{\text{class}}^{n-1} Y_2 + n(n-1) C_{\text{class}}^{n-2} Y_3 + \cdots + R \approx 0 , \quad (44)$$

where Y_i are functions linear in moments including those of order smaller than N , and R contains only moments which are of higher order. This allows one to successively solve the constraints for $n = 1, n = 2$, etc. and discard all constraints arising for $n \geq N + 1$, $n > 0$. In each case, one has to find the terms of lowest order in the moment expansion, in combination with powers C_{class}^n , to see at which order a constraint becomes relevant.

It is crucial for this procedure to work that C_{class}^n , which arises in all constraints, can be eliminated at least for all $n > n'$ through terms of higher order moments using the principal constraint C_Q . This key property can easily be seen to be realized for any non-relativistic particle even in a potential, as long as p_t appears linearly. (For relativistic particles, additional subtleties arise as discussed in a forthcoming paper.) While (64)–(69) change their form in such a case with a different classical constraint, the procedure sketched here still applies. Thus, it does not only refer to quadratic constraints but is sufficiently general for non-relativistic quantum mechanics.

We will explicitly demonstrate the procedure for the free particle in what follows. For that purpose, we rewrote the set of constraints in the required form (44) for moments up to third order as seen in App. A.

6.2 Consistency of constraints for expectation values

At zeroth order, we keep only expectation values. All moments are of order $\mathcal{O}(\lambda^2)$ or higher. As only relevant constraints we therefore find $C^{(n)} \approx 0$, cf. App. A. Keeping only zeroth order terms, this reduces to $C^{(n)} = C_{\text{class}}^n \approx 0$. This in turn corresponds to the single constraint $C_{\text{class}} \approx 0$ which can be used to eliminate p_t in terms of p . The system of constraints is obviously consistent at zeroth order and no constraints on variables associated with the pair (q, p) result.

As explained above, the only constraint that restricts zeroth order moments is $C^{(1)} = C_{\text{class}} \approx 0$. This constraint allows us to eliminate p_t . It generates a gauge flow on expectation values given by

$$\dot{p} = 0 , \quad \dot{p}_t = 0 , \quad \dot{q} = \frac{p}{M} , \quad \dot{t} = 1 . \quad (45)$$

The two observables of the system are therefore

$$\mathcal{P}^{(0)} = p \quad \text{and} \quad \mathcal{Q}^{(0)} = q - t \frac{p}{M} \quad \text{with} \quad \{\mathcal{Q}^{(0)}, \mathcal{P}^{(0)}\} = 1 . \quad (46)$$

These correspond to the two physical degrees of freedom corresponding to expectation values of canonical variables. Among the four original degrees of freedom of the system, p_t is eliminated via the constraint and t is a pure gauge degree of freedom. There are no further constraints to this order, which is thus consistent.

6.3 Consistency of constraints up to second order moments

At second order, we include second order moments and orders of \hbar (recall that \hbar is of order λ^2 in the moment expansion) in addition to expectation values. Third order contributions are set to zero. We find that in addition to $C^{(1)}$, the new constraints $C_q^{(1)}$, $C_t^{(1)}$, $C_{pt}^{(1)}$ and $C_p^{(1)}$ arise. All other constraints are of higher order: Second order moments enter in these equations only through quadratic terms or with a factor of \hbar , both of which are considered as higher order terms, cf. App. A. The only non-trivial constraints are therefore

$$C^{(1)} = C_{\text{class}} + \frac{1}{2M} G_{0,0}^{2,0} \approx 0 \quad (47)$$

$$C_q^{(1)} = G_{1,0}^{0,1} + \frac{p}{M} \frac{i\hbar}{2} + \frac{p}{M} G_{0,0}^{1,1} \approx 0 \quad (48)$$

$$C_t^{(1)} = \frac{p}{M} G_{0,1}^{1,0} + G_{1,1}^{0,0} + \frac{i\hbar}{2} \approx 0 \quad (49)$$

$$C_{pt}^{(1)} = G_{2,0}^{0,0} + \frac{p}{M} G_{1,0}^{1,0} \approx 0 \quad (50)$$

$$C_p^{(1)} = G_{1,0}^{1,0} + \frac{p}{M} G_{0,0}^{2,0} \approx 0, \quad (51)$$

where third order contributions have been set to zero. In accordance with the order of expectation values, we use the first constraint to eliminate $p_t = -p^2/2M - G_{0,0}^{2,0}/2M$ and solve for second order moments

$$\begin{aligned} G_{1,0}^{0,1} &= -\frac{p}{M} \frac{i\hbar}{2} - \frac{p}{M} G_{0,0}^{1,1}, & \frac{p}{M} G_{0,1}^{1,0} &= -G_{1,1}^{0,0} - \frac{i\hbar}{2} \\ G_{2,0}^{0,0} &= -\frac{p}{M} G_{1,0}^{1,0}, & G_{1,0}^{1,0} &= -\frac{p}{M} G_{0,0}^{2,0}. \end{aligned} \quad (52)$$

As constraints for $k > 1$ contain second order moments only through C^n , they are trivial as well. This follows from the first constraint which sets $C^n \sim (G_{0,0}^{2,0})^n \sim \mathcal{O}(\lambda^{2n})$. Thus, as far as the second order moments are concerned, the system of constraints is consistent: $G_{2,0}^{0,0}$, $G_{1,0}^{1,0}$, $G_{0,1}^{1,0}$ and $G_{1,0}^{0,1}$ are fully determined while all second order moments associated with the pair (q, p) can be specified freely. All remaining constraints then determine higher moments. This is the same situation as experienced in the linear case as far as solving the constraints for second order moments is concerned. The inconsistency of Sec. 5.2.2 is avoided because $C^{(3)}$, which made C_{class} and thus $G_{0,0}^{2,0}$ vanish in the sharp truncation, is now realized as a higher order constraint in the moment expansion.

Gauge transformations are generated by $C^{(1)}$, $C_q^{(1)}$, $C_t^{(1)}$, $C_{pt}^{(1)}$ and $C_p^{(1)}$ where third order contributions are set to zero as in (52). In comparison to Sec. 6.2 we have four additional gauge transformations. Whereas $\mathcal{P}^{(2)} := \mathcal{P}^{(0)}$ remains gauge invariant under these transformations as well, this is not the case for $\mathcal{Q}^{(0)}$. The latter has to be alleviated by adding second order moments such that an observable

$$\mathcal{Q}^{(2)} = \mathcal{Q}^{(0)} - \frac{1}{M} G_{0,1}^{1,0} \quad (53)$$

results satisfying $\{\mathcal{Q}^{(2)}, \mathcal{P}^{(2)}\} = 1$.

Calculating the transformations generated by the constraints on second order moments shows that $\mathcal{G}^{pp(2)} = G_{0,0}^{2,0}$ is an observable, i.e. commutes with all five constraints on the hypersurface defined by these constraints. The form of the gauge orbits suggests to make the ansatz

$$\mathcal{G}^{qp(2)} = G_{0,0}^{1,1} + G_{1,1}^{0,0} - \frac{t}{M} G_{0,0}^{2,0} + \frac{i\hbar}{2} \quad (54)$$

$$\mathcal{G}^{qq(2)} = G_{0,0}^{0,2} - 2\frac{p}{M} G_{0,1}^{0,1} + \frac{p^2}{M^2} G_{0,2}^{0,0} - \frac{2t}{M} \left(G_{0,0}^{1,1} + G_{1,1}^{0,0} + \frac{i\hbar}{2} \right) + \frac{t^2}{M^2} G_{0,0}^{2,0} \quad (55)$$

for the remaining two observables. They are invariant under gauge transformations. The term $\frac{i\hbar}{2}$ is included such that the Poisson brackets between $\mathcal{G}^{qq(2)}$ and the remaining two quantum observables are of the required form. They satisfy

$$\{\mathcal{G}^{pp(2)}, \mathcal{G}^{qp(2)}\} = -2\mathcal{G}^{pp(2)} \quad , \quad \{\mathcal{G}^{pp(2)}, \mathcal{G}^{qq(2)}\} = -4\mathcal{G}^{qp(2)} \quad , \quad \{\mathcal{G}^{qp(2)}, \mathcal{G}^{qq(2)}\} = -2\mathcal{G}^{qq(2)} .$$

Commutators between the variables $\mathcal{Q}^{(2)}, \mathcal{P}^{(2)}$ and the physical quantum variables $\mathcal{G}^{qq(2)}, \mathcal{G}^{pp(2)}$ and $\mathcal{G}^{qp(2)}$ vanish.

Thus we showed that four of the ten second order moments are eliminated directly by the constraints. Three of the remaining second order moments, $G_{1,1}^{0,0}$, $G_{0,2}^{0,0}$ and $G_{0,1}^{0,1}$, are pure gauge degrees of freedom. Consequently three physical quantum degrees of freedom remain at second order. The observables can be used to determine the general motion of the system in coordinate time: From (46) and (53) together with (52) and (54) we obtain

$$\begin{aligned} q(t) &= \mathcal{Q}^{(2)} + \frac{t}{M} \mathcal{P}^{(2)} + \frac{1}{M} G_t^p \approx \mathcal{Q}^{(2)} + \frac{t}{M} \mathcal{P}^{(2)} - \frac{1}{p} \left(G_{tp_t} + \frac{i\hbar}{2} \right) \\ &= \mathcal{Q}^{(2)} + \frac{t}{M} \mathcal{P}^{(2)} - \frac{1}{\mathcal{P}^{(2)}} \left(\mathcal{G}^{qp(2)} + \frac{t}{M} \mathcal{G}^{pp(2)} - G^{qp} \right) \end{aligned} \quad (56)$$

for the relational dependence between q , t and G^{qp} . Thus, the moments appear in the solutions for expectation values in coordinate time which illustrates the relation between expectation values and moments. At this stage, we still have to choose a gauge if we want to relate the non-observables q , t and G^{qp} in this equation to properties in a kinematical Hilbert space. A convenient choice is to treat (t, p_t) like a fully constrained pair as we have analyzed it in the example of a linear constraint in Sec. 4. This suggests to fix the gauge by requiring that $G_{tp_t} = -\frac{1}{2}i\hbar$ has no real part but only the imaginary part for physical quantum variables to be real. Moreover, as in the linear case we can gauge fix $G_{tt} = 0$, such that the uncertainty relation $G_{tt}G_{p_t p_t} - (G_{tp_t})^2 \geq \hbar^2/4$ is saturated independently of the behavior of the (q, p) -variables. (For $G_{tt} \neq 0$, it would depend on those variables via $G_{p_t p_t} \approx p^2 G^{pp}/M^2$ from (52).) Finally, this is the only gauge condition for G_{tp_t} which works for all values of $\mathcal{P}^{(2)}$, including $\mathcal{P}^{(2)} = 0$ in (56).

In this gauge, we obtain

$$q(t) = \mathcal{Q}^{(2)} + \frac{\mathcal{P}^{(2)}}{M} t \quad , \quad G^{qp}(t) = \mathcal{G}^{qp(2)} + \frac{\mathcal{G}^{pp(2)}}{M} t \quad (57)$$

in agreement with the solutions one would obtain for the deparameterized free particle. In this case, there is no quantum back-reaction of quantum variables affecting the motion of expectation values because the particle is free. In the presence of a potential, equations analogous to those derived here would exhibit those effects. While it would in general be difficult to determine precise observables in such a case, they can be computed perturbatively starting from the observables found here for the free particle.

6.4 Consistency of constraints up to third order moments

Including third order terms in the analysis, solutions to the constraints $C_q^{(1)}$, $C_t^{(1)}$, $C_{p_t}^{(1)}$ and $C_p^{(1)}$ become

$$G_{1,0}^{0,1} = -\frac{p}{M} \frac{i\hbar}{2} - \frac{p}{M} G_{0,0}^{1,1} - \frac{1}{2M} G_{0,0}^{2,1} \quad (58)$$

$$\frac{p}{M} G_{0,1}^{1,0} = -G_{1,1}^{0,0} - \frac{i\hbar}{2} - \frac{1}{2M} G_{0,1}^{2,0} \quad (59)$$

$$G_{2,0}^{0,0} = -\frac{p}{M} G_{1,0}^{1,0} - \frac{1}{2M} G_{1,0}^{2,0} \quad (60)$$

$$G_{1,0}^{1,0} = -\frac{p}{M} G_{0,0}^{2,0} - \frac{1}{2M} G_{0,0}^{3,0} . \quad (61)$$

As in the previous subsection, they will be used to determine second order moments. The constraint $C^{(1)}$ contains no third order term and thus remains unaltered. Third order moments are determined by higher constraints $C_{qp}^{(1)}$, $C_{tp}^{(1)}$, $C_{p_t p}^{(1)}$, $C_{p^2}^{(1)}$ and $C_q^{(2)}$, $C_t^{(2)}$, $C_{p_t}^{(2)}$. All other constraints contain third order moments with a factor of \hbar or of second or higher moments, both of which provides terms of higher order. For instance, we may consider the constraints $C_{qp^2}^{(1)}$, $C_{tp^2}^{(1)}$, cf. (80), (81). They both contain third order moments with a factor of C_{class} , which, after solving $C^{(1)}$, becomes a term of fifth order. The remaining second and third order terms occur with a factor of \hbar , and are thus of fourth and fifth order. From this consideration of orders in the moment expansion we conclude that $C_{qp^2}^{(1)}$ and $C_{tp^2}^{(1)}$ do not constrain third order moments but become relevant only at higher than third orders of the approximation scheme.

For $n = 1$ the constraints that actually determine third order moments are $C_{qp}^{(1)}$, $C_{tp}^{(1)}$, $C_{p_t p}^{(1)}$ and $C_{p^2}^{(1)}$. On the constraint hypersurface, they imply

$$\begin{aligned} G_{1,0}^{1,1} &\approx -\frac{p}{M} G_{0,0}^{2,1} + \frac{1}{2M} G_{0,0}^{2,0} (G_{0,0}^{1,1} - i\hbar) \quad , \quad G_{1,1}^{1,0} \approx \frac{1}{2M} G_{0,0}^{2,0} G_{0,1}^{1,0} - \frac{p}{M} G_{0,1}^{2,0} \\ G_{2,0}^{1,0} &\approx \frac{1}{2M} G_{0,0}^{2,0} \left(\frac{1}{2M} G_{0,0}^{3,0} + \frac{p}{M} G_{0,0}^{2,0} \right) - \frac{p}{M} G_{1,0}^{2,0} \quad , \quad G_{1,0}^{2,0} \approx \frac{1}{2M} G_{0,0}^{2,0} G_{0,0}^{2,0} - \frac{p}{M} G_{0,0}^{3,0} . \end{aligned}$$

Note that this holds on the constraint hypersurface defined by the constraints $C^{(1)}$, $C_q^{(1)}$, $C_t^{(1)}$, $C_{p_t}^{(1)}$ and $C_p^{(1)}$. Dropping fourth and fifth order terms, we find the simple relations

$$G_{1,0}^{1,1} \approx -\frac{p}{M} G_{0,0}^{2,1} \quad , \quad G_{1,1}^{1,0} \approx -\frac{p}{M} G_{0,1}^{2,0} \quad , \quad G_{2,0}^{1,0} \approx -\frac{p}{M} G_{1,0}^{2,0} \quad , \quad G_{1,0}^{2,0} \approx -\frac{p}{M} G_{0,0}^{3,0} .$$

This happens in a consistent manner because unconstrained third order moments appear on the right hand sides. No condition for the (q, p) -moments appearing here arises in this way, but the third order moments $G_{1,1}^{1,0}$ and $G_{2,1}^{0,0}$ associated with (t, p_t) remain unspecified at this stage. The constraints $C_q^{(2)}$, $C_t^{(2)}$, $C_{p_t}^{(2)}$ arising for $n = 2$ yield

$$\begin{aligned} G_{2,0}^{0,1} &\approx \frac{p}{2M^2} G_{0,0}^{2,0} G_{0,0}^{1,1} \\ G_{2,1}^{0,0} &\approx \frac{1}{M} \left(G_{0,0}^{2,0} \left(G_{1,1}^{0,0} + \frac{1}{2M} G_{0,1}^{2,0} \right) + \frac{p^2}{M} G_{0,1}^{2,0} \right) \\ G_{3,0}^{0,0} &\approx 2 \frac{p}{M} \left(-\frac{p^2}{2M^2} G_{0,0}^{3,0} + \frac{1}{2M} G_{0,0}^{2,0} \left(\frac{1}{2M} G_{0,0}^{3,0} + \frac{p}{2M} G_{0,0}^{2,0} \right) \right), \end{aligned}$$

which, after setting higher order terms to zero, sets

$$G_{2,0}^{0,1} \approx 0 \quad , \quad G_{2,1}^{0,0} \approx \frac{p^2}{M^2} G_{0,1}^{2,0} \quad , \quad G_{3,0}^{0,0} \approx -2 \frac{p^3}{2M^3} G_{0,0}^{3,0}.$$

The inclusion of third order terms and new constraints does not affect $\mathcal{P}^{(2)}$ and $\mathcal{Q}^{(2)}$. They remain constant under gauge transformations. We therefore write

$$\mathcal{P}^{(3)} := \mathcal{P}^{(0)} \quad \text{and} \quad \mathcal{Q}^{(3)} := \mathcal{Q}^{(2)}. \quad (62)$$

Accordingly, their Poisson bracket is unaltered. The situation is different for the second order quantum variables. Only $\mathcal{G}^{pp(2)}$ remains invariant under the flow generated by third order constraints. Now that third order terms are included, $\mathcal{G}^{qp(2)}$ and $\mathcal{G}^{qq(2)}$ are no longer observables. The former transforms under gauge transformations as follows

$$\begin{aligned} \{\mathcal{G}^{qp(2)}, C_q^{(1)}\} &= \frac{1}{2M} G_{0,0}^{2,1} \quad , \quad \{\mathcal{G}^{qp(2)}, C_t^{(1)}\} = \frac{1}{2M} G_{0,1}^{2,0} \\ \{\mathcal{G}^{qp(2)}, C_{p_t}^{(1)}\} &= \frac{1}{2M} G_{1,0}^{2,0} \quad , \quad \{\mathcal{G}^{qp(2)}, C_p^{(1)}\} = \frac{1}{2M} G_{0,0}^{3,0} \end{aligned}$$

whereas Poisson brackets with $C_{qp}^{(1)}$, $C_{tp}^{(1)}$, $C_{p,p}^{(1)}$ and $C_{p^2}^{(1)}$ are of fourth order in the moment expansion. The terms on the right hand side can be eliminated through the addition of a third order moment by

$$\mathcal{G}^{qp(3)} := \mathcal{G}^{qp(2)} - \frac{1}{2M} G_{0,1}^{2,0}. \quad (63)$$

This has vanishing Poisson brackets with all constraints up to fourth order terms. Moreover, it has vanishing Poisson bracket with $\mathcal{P}^{(3)}$ as well as $\mathcal{Q}^{(3)}$. The Poisson bracket with $\mathcal{G}^{pp(3)} := \mathcal{G}^{pp(2)}$ remains unaltered, $\{\mathcal{G}^{qp(3)}, \mathcal{G}^{pp(3)}\} = 2\mathcal{G}^{pp(3)}$.

The transformations generated by the constraints on $\mathcal{G}^{qq(2)}$ are of a more complicated form and we have not found a simple way of writing $\mathcal{G}^{qq(3)}$ in explicit form. We conclude at this place because the applicability of effective constraints has been demonstrated. As already mentioned, the procedure also applies to interacting systems: We can solve the constraints in the same manner and using the same orders of constraints. The main consequence in the presence of a potential $V(q)$ is that additional q -moments appear as extra terms in solutions at certain orders, whose precise form depends on the potential. For a small potential, this can be dealt with by perturbation theory around the free solutions.

7 Conclusions

We have introduced an effective procedure to treat constrained systems, which demonstrates how many of the technical and conceptual problems arising otherwise in those cases can be avoided or overcome. The procedure applies equally well to constraints with zero in the discrete or continuous parts of their spectra and is, in fact, independent of many representation properties. For each classical constraint, infinitely many constraints are imposed on an infinite-dimensional quantum phase space comprised of expectation values and moments of states. This system is manageable when solved order by order in the moments because this requires the consideration of only finitely many constraints at each order. A formal definition of this moment expansion has been given in Sec. 6.1.

The principal constraint is simply the expectation value $C_Q = \langle \hat{C} \rangle$ of a constraint operator, viewed as a function of moments via the state used. Unless the constraint is linear, there are quantum corrections depending on moments which can be analyzed for physical implications. Moments are themselves subject to further constraints, thus restricting the form of quantum corrections in C_Q .

We have demonstrated that there is a consistent procedure in which an expansion by moments can be defined, in analogy with an expansion by moments in effective equations for unconstrained systems. This has been shown to be applicable to any parameterized non-relativistic system. We have also demonstrated the procedure with explicit calculations in a simple example corresponding to the parameterized free non-relativistic particle. In these cases, when faced with infinitely many constraints we could explicitly choose an internal time variable and eliminate all its associated moments to the orders considered. Especially for the free particle, we were able to determine observables invariant under the flows generated by the constraints, and more generally observed how such equations encode quantum back-reaction of moments on expectation values in an interacting system. These observables were subjected to reality conditions to ensure that they correspond to expectation values and moments computed in a state of the *physical Hilbert space*. Especially physical Hilbert space issues appear much simpler in this framework compared to a direct treatment, being imposed just by reality conditions for functions rather than self-adjointness conditions for operators. Nevertheless, crucial properties of the physical Hilbert space are still recognizable despite of the fact that we do not refer to a specific quantum representation. We also emphasize that we choose an internal time after quantization, because we do so when evaluating effective constraints obtained from expectation values of operators. This is a new feature which may allow new concepts of emergent times given by quantum variables even in situations where no classical internal time would be available (see e.g. [19]).

In the examples, we have explicitly implemented the physical Hilbert space by reality conditions on observables given by physical expectation values and physical quantum variables. Observables thus play important roles and techniques of [26, 27, 28] might prove useful in this context. Notice that we are referring to observables of the quantum theory, although they formally appear as observables in a classical-type theory of infinitely many constraints for infinitely many variables. The fact that it often suffices to compute these

observables order by order in the moment expansion greatly simplifies the computation of observables of the quantum theory. Nevertheless, especially for gravitational systems of sufficiently large complexity one does not even expect classical observables to be computable in explicit form. Then, additional expansions such as cosmological perturbations can be combined with the moment expansion to make calculations feasible. This provides almost all applications of interest. Moreover, if observables cannot be determined completely, gauge fixing conditions can be used. As we observed, depending on the specific gauge fixing some of the kinematical quantum variables (before imposing constraints) can be complex-valued while the final physical variables are required to be real. Different gauge fixings imply different kinematical reality conditions, which can be understood as different kinematical Hilbert space structures all resulting in the same physical Hilbert space.

While we have discussed only the simplest examples, this led us to introduce approximation schemes which are suitable more generally. In more complicated systems such as quantum cosmology one may not be able to find, e.g., explicit expressions for physical quantum variables as complete observables. But for effective equations it is sufficient to know the local behavior of gauge-invariant quantities, which can then be connected to long-term trajectories obtained by solving effective equations. A local treatment, on the other hand, allows one to linearize gauge orbits, making it possible to determine observables. Moreover, as always in the context of effective equations, simple models can serve as a basis for perturbation theories of more complicated systems.

A class of systems of particular interest is given by quantum cosmology as an example for parameterized relativistic systems to be discussed in a forthcoming paper. In such a case, the linear term p_t in the systems considered here would be replaced by a square p_t^2 . There is thus a sign ambiguity in p_t which has some subtle implications. Moreover, the principal quantum constraint C_Q will then acquire an additional moment $G_{p_t p_t}$ which may spoil the suitability of t as internal time in quantum theory provided that the fluctuation $G_{p_t p_t}$ can become large enough for no real solution for p_t to exist. This demonstrates a further advantage of the effective constraint formalism which we have not elaborated here: the self-consistency of emergent time pictures can be analyzed directly from the structure of equations. Finally, if there are several classical constraints, anomaly issues can be analyzed at the effective level without many of the intricacies arising for constraint operators. Also this will be discussed in more detail elsewhere [8].

To summarize, we have seen that the principal constraint C_Q already provides quantum corrections on the classical constrained variables. The procedure thus promises a manageable route to derive corrections from, e.g., quantum gravity in a way in which physical reality conditions can be implemented. Since such conditions can be imposed order by order in moments as well as other perturbations, results can be arrived at much more easily compared to the computation of full physical states in a Hilbert space. Nevertheless, all physical requirements are implemented.

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A System of constraints for the parametrized free particle

General expression for the constraints are

$$C^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} p_t^{m-j} \frac{p^{2(n-m)-\ell}}{(2M)^{n-m}} G_{j,0}^{\ell,0} \quad (64)$$

$$C_q^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} p_t^{m-j} \frac{p^{2(n-m)-\ell}}{(2M)^{n-m}} \left(q G_{j,0}^{\ell,0} + G_{j,0}^{\ell,1} + \frac{i\hbar}{2} \ell G_{j,0}^{\ell-1,0} \right)$$

$$C_t^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} p_t^{m-j} \frac{p^{2(n-m)-\ell}}{(2M)^{n-m}} \left(t G_{j,0}^{\ell,0} + G_{j,1}^{\ell,0} + \frac{i\hbar}{2} j G_{j-1,0}^{\ell,0} \right)$$

$$C_{p_t}^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} p_t^{m-j} \frac{p^{2(n-m)-\ell}}{(2M)^{n-m}} \left(p_t G_{j,0}^{\ell,0} + G_{j+1,0}^{\ell,0} \right) \quad (65)$$

$$C_{p^k}^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \sum_{r=0}^k \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} \binom{k}{r} p_t^{m-j} \frac{p^{2(n-m)+k-\ell-r}}{(2M)^{n-m}} G_{j,0}^{\ell+r,0} \quad (66)$$

$$C_{tp^k}^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \sum_{r=0}^k \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} \binom{k}{r} p_t^{m-j} \frac{p^{2(n-m)+k-\ell-r}}{(2M)^{n-m}} \times \left(t G_{j,0}^{\ell+r,0} + G_{j,1}^{\ell+r,0} + \frac{i\hbar}{2} j G_{j-1,0}^{\ell+r,0} \right) \quad (67)$$

$$C_{qp^k}^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \sum_{r=0}^k \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} \binom{k}{r} p_t^{m-j} \frac{p^{2(n-m)+k-\ell-r}}{(2M)^{n-m}} \times \left(q G_{j,0}^{\ell+r,0} + G_{j,0}^{\ell+r,1} + \frac{i\hbar}{2} (\ell+r) G_{j,0}^{\ell+r-1,0} \right) \quad (68)$$

$$C_{p_t p^k}^{(n)} = \sum_{m=0}^n \sum_{j=0}^m \sum_{\ell=0}^{2(n-m)} \sum_{r=0}^k \binom{n}{m} \binom{m}{j} \binom{2(n-m)}{\ell} \binom{k}{r} p_t^{m-j} \frac{p^{2(n-m)+k-\ell-r}}{(2M)^{n-m}} \times \left(p_t G_{j,0}^{\ell+r,0} + G_{j+1,0}^{\ell+r,0} \right) . \quad (69)$$

In addition to those written explicitly here, there are those involving higher polynomials also in q , t and p_t . The first two types of those constraints are more lengthy due to

reorderings in the quantum variables. The constraints listed suffice for considerations in this paper.

In a moment expansion, the leading terms of these constraints are

$$\begin{aligned}
C^{(n)} &= C_{\text{class}}^n + nC_{\text{class}}^{n-1} \frac{1}{2M} G_{0,0}^{2,0} \\
&+ n(n-1)C_{\text{class}}^{n-2} \left[\frac{p^2}{2M^2} G_{0,0}^{2,0} + \frac{p}{M} G_{1,0}^{1,0} + \frac{1}{2} G_{2,0}^{0,0} + \frac{1}{2M} G_{1,0}^{2,0} + \frac{p}{2M^2} G_{0,0}^{3,0} + \frac{1}{8M^2} G_{0,0}^{4,0} \right] \\
&+ n(n-1)(n-2)C_{\text{class}}^{n-3} \left[\frac{p^2}{2M^2} G_{1,0}^{2,0} + \frac{p}{2M} G_{2,0}^{1,0} + \frac{1}{6} G_{3,0}^{0,0} + \frac{p^3}{6M^3} G_{0,0}^{3,0} + X_1 \right] \\
&+ n(n-1)(n-2)(n-3)R_1 = 0
\end{aligned} \tag{70}$$

$$\begin{aligned}
C_q^{(n)} &= qC^{(n)} + nC_{\text{class}}^{n-1} \left[\frac{p}{M} \frac{i\hbar}{2} + \frac{p}{M} G_{0,0}^{1,1} + G_{1,0}^{0,1} + \frac{1}{2M} G_{0,0}^{2,1} \right] \\
&+ n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \frac{1}{M} \left(G_{1,0}^{1,0} + \frac{3p}{2M} G_{0,0}^{2,0} \right) + \frac{p^2}{2M^2} G_{0,0}^{2,1} + \frac{p}{M} G_{1,0}^{1,1} + \frac{1}{2} G_{2,0}^{0,1} + \frac{i\hbar}{2} \frac{1}{2M^2} G_{0,0}^{3,0} + X_2 \right] \\
&+ n(n-1)(n-2)C_{\text{class}}^{n-3} \left[\frac{i\hbar}{2} \left(\frac{p^2}{M^2} G_{1,0}^{1,0} + \frac{p^3}{2M^3} G_{0,0}^{2,0} + \frac{p}{2M} G_{2,0}^{0,0} + \frac{3p}{2M^2} G_{1,0}^{2,0} + \frac{p^2}{M^3} G_{0,0}^{3,0} + \frac{1}{2M} G_{2,0}^{1,0} \right) + X_3 \right] \\
&+ n(n-1)(n-2)(n-3)C_{\text{class}}^{n-4} \left[\frac{i\hbar}{2} \left(\frac{p^4}{6M^4} G_{0,0}^{3,0} + \frac{p^3}{2M^3} G_{1,0}^{2,0} + \frac{p^2}{2M^2} G_{2,0}^{1,0} + \frac{p}{6M} G_{3,0}^{0,0} \right) + X_4 \right] \\
&+ n(n-1)(n-2)(n-3)(n-4)R_2 = 0
\end{aligned} \tag{71}$$

$$\begin{aligned}
C_t^{(n)} &= tC^{(n)} + nC_{\text{class}}^{n-1} \left[\frac{i\hbar}{2} + \frac{p}{M} G_{0,1}^{1,0} + G_{1,1}^{0,0} + \frac{1}{2M} G_{0,1}^{2,0} \right] \\
&+ n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \frac{1}{2M} G_{0,0}^{2,0} + \frac{p^2}{2M^2} G_{0,1}^{2,0} + \frac{p}{M} G_{1,1}^{1,0} + \frac{1}{2} G_{2,1}^{0,0} + X_5 \right] \\
&+ n(n-1)(n-2)C_{\text{class}}^{n-3} \left[\frac{i\hbar}{2} \left(\frac{p}{M} G_{1,0}^{1,0} + \frac{1}{2} G_{2,0}^{0,0} + \frac{p^2}{2M^2} G_{0,0}^{2,0} + \frac{p}{2M^2} G_{0,0}^{3,0} + \frac{1}{2M} G_{1,0}^{2,0} \right) + X_6 \right] \\
&+ n(n-1)(n-2)(n-3)C_{\text{class}}^{n-4} \left[\frac{i\hbar}{2} \left(\frac{p^3}{6M^3} G_{0,0}^{3,0} + \frac{p^2}{2M^2} G_{1,0}^{2,0} + \frac{p}{2M} G_{2,0}^{1,0} + \frac{1}{6} G_{3,0}^{0,0} \right) + X_7 \right] \\
&+ n(n-1)(n-2)(n-3)(n-4)R_3 = 0
\end{aligned} \tag{72}$$

$$\begin{aligned}
C_{p_t}^{(n)} &= p_t C^{(n)} + nC_{\text{class}}^{n-1} \left[\frac{p}{M} G_{1,0}^{1,0} + G_{2,0}^{0,0} + \frac{1}{2M} G_{1,0}^{2,0} \right] \\
&+ n(n-1)C_{\text{class}}^{n-2} \left[\frac{p^2}{2M^2} G_{1,0}^{2,0} + \frac{p}{M} G_{2,0}^{1,0} + \frac{1}{2} G_{3,0}^{0,0} + X_8 \right] \\
&+ n(n-1)(n-2)R_4 = 0
\end{aligned} \tag{73}$$

$$\begin{aligned}
C_p^{(n)} &= pC^{(n)} + nC_{\text{class}}^{n-1} \left[G_{1,0}^{1,0} + \frac{1}{2M} G_{0,0}^{3,0} + \frac{p}{M} G_{0,0}^{2,0} \right] \\
&+ n(n-1)C_{\text{class}}^{n-2} \left[\frac{p^2}{2M^2} G_{0,0}^{3,0} + \frac{p}{M} G_{1,0}^{2,0} + \frac{1}{2} G_{2,0}^{1,0} + X_9 \right] \\
&+ n(n-1)(n-2)R_5 = 0
\end{aligned} \tag{74}$$

$$C_{p^2}^{(n)} = 2pC_p^{(n)} - pC^{(n)} + C_{\text{class}}^n G_{0,0}^{2,0} + nC_{\text{class}}^{n-1} \left[\frac{p}{M} G_{0,0}^{3,0} + G_{1,0}^{2,0} + \frac{1}{2M} G_{0,0}^{4,0} \right] + n(n-1)R_6 = 0 \tag{75}$$

$$\begin{aligned}
C_{tp}^{(n)} &= tC_p^{(n)} + pC_t^{(n)} + C_{\text{class}}^n G_{0,1}^{1,0} + nC_{\text{class}}^{n-1} \left[\frac{p}{M} G_{0,1}^{2,0} + \frac{1}{2M} G_{0,1}^{3,0} + G_{1,1}^{1,0} \right] \\
&\quad + n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \left(\frac{p}{M} G_{0,0}^{2,0} + G_{1,0}^{1,0} + \frac{1}{2M} G_{0,0}^{3,0} \right) + X_{10} \right] \\
&\quad + n(n-1)(n-2)C_{\text{class}}^{n-3} \left[\frac{i\hbar}{2} \left(\frac{p^2}{2M^2} G_{0,0}^{3,0} + \frac{1}{2} G_{2,0}^{1,0} + \frac{p}{M} G_{1,0}^{2,0} \right) + X_{11} \right] \\
&\quad + n(n-1)(n-2)(n-3)R_7 = 0
\end{aligned} \tag{76}$$

$$\begin{aligned}
C_{qp}^{(n)} &= qC_p^{(n)} + pC_q^{(n)} + C_{\text{class}}^n \left[G_{0,0}^{1,1} + \frac{i\hbar}{2} \right] \\
&\quad + nC_{\text{class}}^{n-1} \left[3\frac{i\hbar}{2} \frac{1}{2M} G_{0,0}^{2,0} + \frac{p}{M} G_{0,0}^{2,1} + G_{1,0}^{1,1} + \frac{1}{2M} G_{0,0}^{3,1} \right] \\
&\quad + n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \left(\frac{3p^2}{2M^2} G_{0,0}^{2,0} + \frac{2p}{M} G_{1,0}^{1,0} + \frac{1}{2} G_{2,0}^{0,0} + \frac{2p}{M^2} G_{0,0}^{3,0} + \frac{3}{2M} G_{1,0}^{2,0} \right) + X_{12} \right] \\
&\quad + n(n-1)(n-2)C_{\text{class}}^{n-3} \left[\frac{i\hbar}{2} \left(\frac{3p^2}{2M^2} G_{1,0}^{2,0} + \frac{2p^3}{3M^3} G_{0,0}^{3,0} + \frac{p}{M} G_{2,0}^{1,0} + \frac{1}{6} G_{3,0}^{0,0} \right) + X_{13} \right] \\
&\quad + n(n-1)(n-2)(n-3)R_8 = 0
\end{aligned} \tag{77}$$

$$C_{ptp}^{(n)} = p_t C_p^{(n)} + p C_{p_t}^{(n)} + C_{\text{class}}^n G_{1,0}^{1,0} + nC_{\text{class}}^{n-1} \left[\frac{p}{M} G_{1,0}^{2,0} + G_{2,0}^{1,0} + \frac{1}{2M} G_{1,0}^{3,0} \right] + n(n-1)R_9 = 0 \tag{78}$$

$$C_{p^3}^{(n)} = 3pC_{p^2}^{(n)} - 3p^2C_p^{(n)} + p^3C^{(n)} + C_{\text{class}}^n G_{0,0}^{3,0} + nC_{\text{class}}^{n-1} X_{14} + n(n-1)R_{10} = 0 \tag{79}$$

$$\begin{aligned}
C_{tp^2}^{(n)} &= tC_{p^2}^{(n)} - p^2C_t^{(n)} + 2pC_{tp}^{(n)} - 2ptC_p^{(n)} \\
&\quad + C_{\text{class}}^n G_{0,1}^{2,0} + nC_{\text{class}}^{n-1} \left[\frac{i\hbar}{2} G_{0,0}^{2,0} + X_{15} \right] \\
&\quad + n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \left(\frac{p}{M} G_{0,0}^{3,0} + G_{1,0}^{2,0} \right) + X_{16} \right] \\
&\quad + n(n-1)(n-2)R_{11} = 0
\end{aligned} \tag{80}$$

$$\begin{aligned}
C_{qp^2}^{(n)} &= qC_{p^2}^{(n)} - p^2C_q^{(n)} + 2pC_{qp}^{(n)} - 2pqC_p^{(n)} \\
&\quad + C_{\text{class}}^n G_{0,0}^{2,1} + nC_{\text{class}}^{n-1} \left[\frac{i\hbar}{2} \left(3\frac{p}{M} G_{0,0}^{2,0} + 2G_{1,0}^{1,0} + 4\frac{1}{2M} G_{0,0}^{3,0} \right) + X_{17} \right] \\
&\quad + n(n-1)C_{\text{class}}^{n-2} \left[\frac{i\hbar}{2} \left(\frac{2p^2}{M^2} G_{0,0}^{3,0} + 3\frac{p}{M} G_{1,0}^{2,0} + G_{2,0}^{1,0} \right) + X_{18} \right] \\
&\quad + n(n-1)(n-2)R_{12} = 0
\end{aligned} \tag{81}$$

$$\begin{aligned}
C_{ptp^2}^{(n)} &= p_t C_{p^2}^{(n)} - p^2 C_{p_t}^{(n)} + 2p C_{p_t p}^{(n)} - 2p p_t C_p^{(n)} \\
&\quad + C_{\text{class}}^n G_{1,0}^{2,0} + nC_{\text{class}}^{n-1} X_{19} + n(n-1)R_{13} = 0
\end{aligned} \tag{82}$$

$$\begin{aligned}
C_{tp^3}^{(n)} &= tC_{p^3}^{(n)} + p^3C_t^{(n)} - 3p^2C_{tp}^{(n)} + 3^2ptC_p^{(n)} + 3pC_{tp^2}^{(n)} - 3ptC_{p^2}^{(n)} \\
&\quad + C_{\text{class}}^n G_{0,1}^{3,0} + nC_{\text{class}}^{n-1} \left[\frac{i\hbar}{2} G_{0,0}^{3,0} + X_{20} \right] + n(n-1)R_{14} = 0
\end{aligned} \tag{83}$$

$$C_{qp^3}^{(n)} = qC_{p^3}^{(n)} + p^3C_q^{(n)} - 3p^2C_{qp}^{(n)} + 3^2pqC_p^{(n)} + 3pC_{qp^2}^{(n)} - 3pqC_{p^2}^{(n)}$$

$$\begin{aligned}
& + C_{\text{class}}^n \left[G_{0,0}^{3,1} + 3 \frac{i\hbar}{2} G_{0,0}^{2,0} \right] \\
& + n C_{\text{class}}^{n-1} \left[\frac{i\hbar}{2} \left(4 \frac{p}{M} G_{0,0}^{3,0} + 3 G_{1,0}^{2,0} \right) + X_{21} \right] + n(n-1) R_{15} = 0 ,
\end{aligned} \tag{84}$$

where X_i and R_i are linear functions of higher, i.e. at least fourth, order moments.

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